Oak Ridge National Laboratory's Neutron Sciences

10-Year SNS-HFIR Beamline Roadmap

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OAK RIDGE National Laboratory | HIGH FLUX ISOTOPE REACTOR | SPALLATION NEUTRON SOURCE

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Executive Summary

The Neutron Sciences Directorate at Oak Ridge National Laboratory (ORNL) operates two neutron scattering scientific user facilities—the High Flux Isotope Reactor (HFIR) and the Spallation Neutron Source (SNS)—for the US Department of Energy (DOE) Office of Science. The Directorate is committed to providing diverse and world-class neutron scattering and imaging instrumentation and associated capabilities to enable the most impactful research by the scientific community.

The *10-year Beamline Roadmap* has been developed in response to a specific action item from the 2023 DOE Operations Review of HFIR and SNS:

> *Create a 10-year SNS-HFIR beamline roadmap with instrument retirements and replacements, refurbishments, upgrades, and prioritizations, which focuses on maximizing the facilities' scientific output, optimizing the use of each source, and growing the user base. The beamline roadmap together with its implementation plan and milestones should be submitted to BES by the end of FY 2024.*

Most of this document directly responds to that action item. Additionally, the document includes two perspectives on the longer-term future of the instrument suite at SNS and HFIR. The first describes possible instruments at the Second Target Station and the implications of this suite on the current instruments at SNS and HFIR, and the second describes possible instruments that could be developed if new thermal and cold guide halls at HFIR were prioritized after the completion of the Pressure Vessel Replacement (PVR) project.

As described in detail herein, our instrument plans are developed based on various sources of community feedback and discussed with our neutron user community. Approximately every three years, we organize instrument suite assessments during which plans for instrument upgrades, new instruments, staffing, sample environment developments, and software developments are discussed with a review committee composed of both facility experts and representatives from the user community. The first set of these assessments occurred in 2016–2017. To-date, two suite assessments have occurred, and another set is planned for FY 2025. These assessments produce recommendation reports, including prioritization, for each instrument suite. We have also utilized ad hoc, focused review committees such as the Instrument Advisory Board (IAB) and the HFIR Prioritization Advisory Committee (HIPAC). As discussed in this document, the recommendations from the IAB played an important role in developing our facility plans, and the HIPAC report led to the formation of an internal HFIR Beam Room Optimization Working Group to address the specific recommendations of this committee.

This document details three new instrument concepts that have mature technical designs that have been developed in consultation with the user community:

1. ***IMAGINE-X*** (CG-4D and later NB-1 at HFIR)—integration of dynamic nuclear polarization and addition of field-insensitive Anger cameras will enable macromolecular crystallography with significantly enhanced sensitivity for determining hydrogen locations.
2. ***DISCOVER*** (BL-8A at SNS)—a medium-resolution powder diffractometer capable of simultaneous diffraction and high-fidelity pair distribution function (PDF) measurements.
3. ***MANTA*** (NB-6 at HFIR)—a modern cold neutron triple-axis spectrometer with a multi-analyzer secondary spectrometer.

IMAGINE-X has been funded via the US Department of Energy (DOE) Biopreparedness Research Virtual Environment (BRaVE) initiative. External funding is actively being sought for DISCOVER. The primary spectrometer and infrastructure to enable multiple secondary spectrometers for MANTA will be funded via the Accelerator Improvement Project (AIP) mechanism. The full multi-analyzer secondary spectrometer for MANTA will require additional funding. Another new instrument concept, the HFIR neutron spin echo (NSE) spectrometer, has been discussed in detail with the community. Some remaining open questions about the design and performance of this instrument require more focused development activities.

Several other instrument concepts are described in this document (e.g., MICRON, CERBERUS, SESANS). These instruments have been designed to provide complementary capabilities and to address gaps in our current instrument suite but with consideration of the constrained space afforded by shared beam ports at SNS. These concepts should be viewed as preliminary in nature and have, generally, been discussed in less detail with the user community.

Some opportunities for relocation of instruments are also discussed in this document:

1. Relocation of MARS to NB-4 following the HFIR Beryllium Reflector Replacement (HBRR)
2. Relocation of USANS (BL-1A at SNS) to HFIR
3. Possible reconfiguration to enable the addition of a high-resolution powder diffractometer
4. Options for BL-15 following the completion of the HFIR neutron spin echo spectrometer

Although all instruments in the HFIR cold guide hall will be relocated slightly during the HBRR activity because of the transition from a four-guide network to a six-guide network, MARS will experience the most significant disruption. This instrument will be moved from the current CG-1 beamline to a location between the GP-SANS and Bio-SANS instruments and will be enabled by the HFIR cold guide hall extension. Of the remaining potential relocations, the most feasible is relocation of USANS, and an internal working group has been established to estimate performance and make a recommendation to management. This potential relocation has also been discussed with the HBRR team to ensure integration with their activity. Working groups will be established to consider options to enable addition of a high-resolution powder diffractometer and to develop a comprehensive strategy for optimizing neutron spin echo instruments across SNS (First and Second target stations) and HFIR.

Significant performance improvements and additional capabilities can be added by means of instrument upgrades, and a well-established process for prioritizing and executing these upgrades exists. Upgrades described in this document include recently completed upgrades, ongoing funded upgrades, concepts that are prioritized but not currently funded, concepts that were considered but are not currently prioritized, and longer-term instrument upgrades that could require significant R&D.

Community Engagement

An important next step is socializing the *10-Year Beamline Roadmap* with the user community. Instrument suite assessments will be held in FY 2025 which will concentrate on the plans described in this document and will serve as important community feedback. Following this, we will reconstitute the IAB to provide broader, facility-level feedback on these plans. To more broadly discuss the beamline roadmap with the user community, we will hold webinars. Finally, activities are ongoing to refine the science case and reconsider the initial instrument suite for STS in response to feedback from the Basic Energy Sciences Advisory Committee. A modified instrument suite for STS could affect the longer-term instrument plans discussed in this report, and the identified science needs could lead to changes in priorities for current SNS and HFIR instruments. This information will be incorporated into instrument planning once it is available. Feedback on plan revisions and discussion of progress will be obtained periodically from the user community. As summarized in Table 1, opportunities for community feedback include the SNS–HFIR User Group meeting, American Conference on Neutron Scattering, the International Conference on Neutron scattering, and focused technique workshops. The beamline road map will be a living document, so we will update it as plans evolve and activities are completed.

Table 1. Summary of opportunities for discussion of the beamline roadmap and progress with the user community.

Review of the *10-Year Beamline Roadmap*	
FY 2025	Instrument suite assessments
FY 2025	Instrument Advisory Board
FY 2025	Webinars to discuss the roadmap with the broader community
Ongoing community engagement activities to discuss plans and progress	
2026, ’28, ’30, ’32, ’34	American Conference on Neutron Scattering
2025, ’27, ’29, ’31, ’33	SNS–HFIR User Group meeting
2025, ’29, ’34	International Conference on Neutron Scattering
2025, ’28, ’31, ’34	Instrument suite assessments
All years	Technique-specific workshops
All years	Webinars and town hall meetings to discuss plans and progress
All years	Update the roadmap

Introduction

This document provides a roadmap for existing and potential new instruments at the Spallation Neutron Source (SNS) and the High Flux Isotope Reactor (HFIR). The information herein was assembled through an internal process that was guided and influenced by interactions with the user community and observed scientific trends. A high-level summary and timeline of the roadmap is included in Figure 1. This document describes not only prioritized plans for new instruments, relocations, and upgrades but also the decision-making processes. The “Introduction” section of the document includes a set of assumptions and provides brief descriptions of each instrument at SNS and HFIR to serve as background information. The “Prioritization Processes” section describes how we obtain information from the user and broader scientific communities and develop plans guided by this feedback. This section also describes the internal processes for decision-making and prioritization, and external reviews to evaluate progress and plans. Also included are details of the roadmap, which is organized into a high-level section describing new instruments or relocations at SNS and then HFIR and followed by a section describing instrument upgrades. Finally, two longer-term perspectives are included. The first describes the instrument suite that could be available following completion of the Second Target Station (STS) and the potential impact of these instruments on the current suite. The second describes a much longer-term possibility for an expanded HFIR instrument suite if additional thermal and cold guide halls were constructed following completion of the Pressure Vessel Replacement (PVR) project.

Assumptions

The plans described herein are guided by future opportunities for instrument suite expansion and consideration of the national landscape for neutron instrumentation. For this document, we assume the STS project is completed in the mid to late 2030s. The instrument suite for STS will be developed in the context of considering the strengths of the three sources (HFIR, SNS First Target Station [FTS] and STS). Another consequential situation within the US research community is the status of the National Institute of Standards and Technology Center for Neutron Research (NCNR). This facility has been shut down since early 2021. The US Nuclear Regulatory Commission has authorized restart of the reactor, but, as of September 2024, no clear timeline has been established for reactor restart. NCNR provides a large suite of instruments for the US neutron scattering community, and this loss of capacity is detrimental. For the purposes of this document, we assume that NCNR will resume operation soon and that this operation will be at the full 20 MW reactor power. Changes to either the operating power or the long-term future of NCNR may alter the prioritization discussed in this document.

Additionally, PVR presents an exciting opportunity for expanding the suite of neutron scattering instruments at HFIR. This activity can enable beam tube reconfiguration and the potential addition of a new cold source. Opportunities exist for adding both a thermal and a cold guide hall at HFIR, significantly increasing capabilities and capacity for neutron scattering. We have added a section to this document that outlines what could be enabled by such guide halls. Ideas for potential instruments in these new guide halls are notional at this point and have not been discussed with the broader user community. These possibilities are presented to provide a perspective on what may be achievable with an expanded HFIR instrument suite.

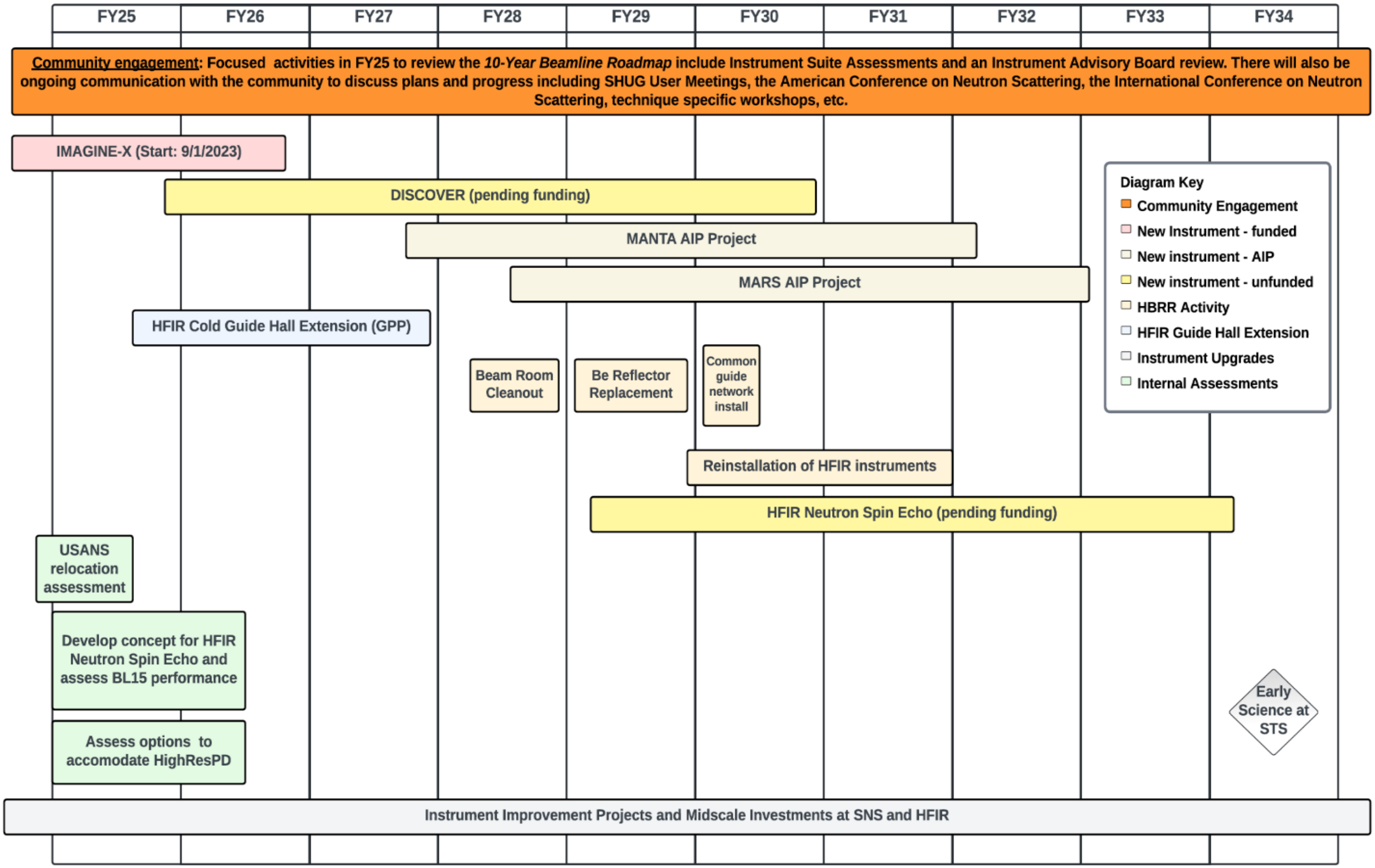


Figure 1. High-level summary of the 10-Year Beamline Roadmap.

This document focuses on the suite of neutron scattering and imaging instruments. Other plans have been developed for sample environment, scientific computing, and user community development, and these plans are not included in this roadmap. Consequently, this document does not discuss activities such as remote experiments, automation, experiment steering, or artificial intelligence. These activities are a high priority for SNS and HFIR, and significant investments in these areas are prioritized using the methods described in this document.

Current SNS and HFIR Instrument Suites

The recently developed *Neutron Sciences 10-Year Strategic Plan* describes a vision for future science challenges where ORNL's neutron sciences facilities can be influential. In that strategic plan, specific challenges were identified in the following areas: quantum materials, soft matter and polymers, materials and engineering, chemistry and environmental science, and biological materials and systems.

The current instrument suites at SNS and HFIR provide a strong set of capabilities in these areas. Tables 2 and 3 map these instruments onto the science areas.

Table 2. List of SNS instruments and their alignment with different science areas.

		Quantum materials	Soft matter and polymers	Materials and engineering	Chemistry and environmental science	Biological materials and systems
SNS Instruments						
Diffractometers	NOMAD (BL-1B)			X	X	
	SNAP (BL-3)	X		X	X	
	VULCAN (BL-7)			X		
	CORELLI (BL-9)	X			X	
	MaNDi (BL-11B)					X
	POWGEN (BL-11A)	X	X	X	X	
	TOPAZ (BL-12)	X		X	X	
Spectrometers	BASIS (BL-2)		X		X	X
	CNCS (BL-5)	X	X		X	X
	HYSPEC (BL-14B)	X				
	NSE (BL-15)		X			X
	VISION (BL-16B)				X	X
	SEQUOIA (BL-17)	X			X	
	ARCS (BL-18)	X				
Small-angle neutron scattering	EQ-SANS (BL-6)		X	X	X	X
	USANS (BL-1A)		X			X
Reflectometers	MAGREF (BL-4A)	X				
	LIQREF (BL-4B)		X	X	X	X
Imaging	VENUS (BL-10)			X	X	X

Table 3. List of HFIR instruments and their alignment with different science areas.

		Quantum materials	Soft matter and polymers	Materials and engineering	Chemistry and environmental science	Biological materials and systems
HFIR Instruments						
Diffractometers	POWDER (HB-2A)	X			X	
	WAND^2 (HB-2C)	X		X	X	X
	HIDRA (HB-2B)			X		
	DEMAND (HB-3A)	X				
	IMAGINE (CG-4D)					X
Spectrometers	VERITAS (HB-1A)	X			X	
	PTAX (HB-1)	X				
	TAX (HB-3)	X			X	
	CTAX (CG-4C)	X			X	
Small-angle neutron scattering	GP-SANS (CG-2)	X	X	X	X	X
	Bio-SANS (CG-3)		X			X
Imaging	MARS (CG-1D)		X	X	X	X

The next section describes the current instruments at SNS and HFIR. These descriptions serve as a reference for later discussions of new instruments, instrument relocations, and instrument upgrades.

Current SNS Instrument Suite

Figure 2 shows a layout of SNS instrument which are described below, grouped by instrument suite.

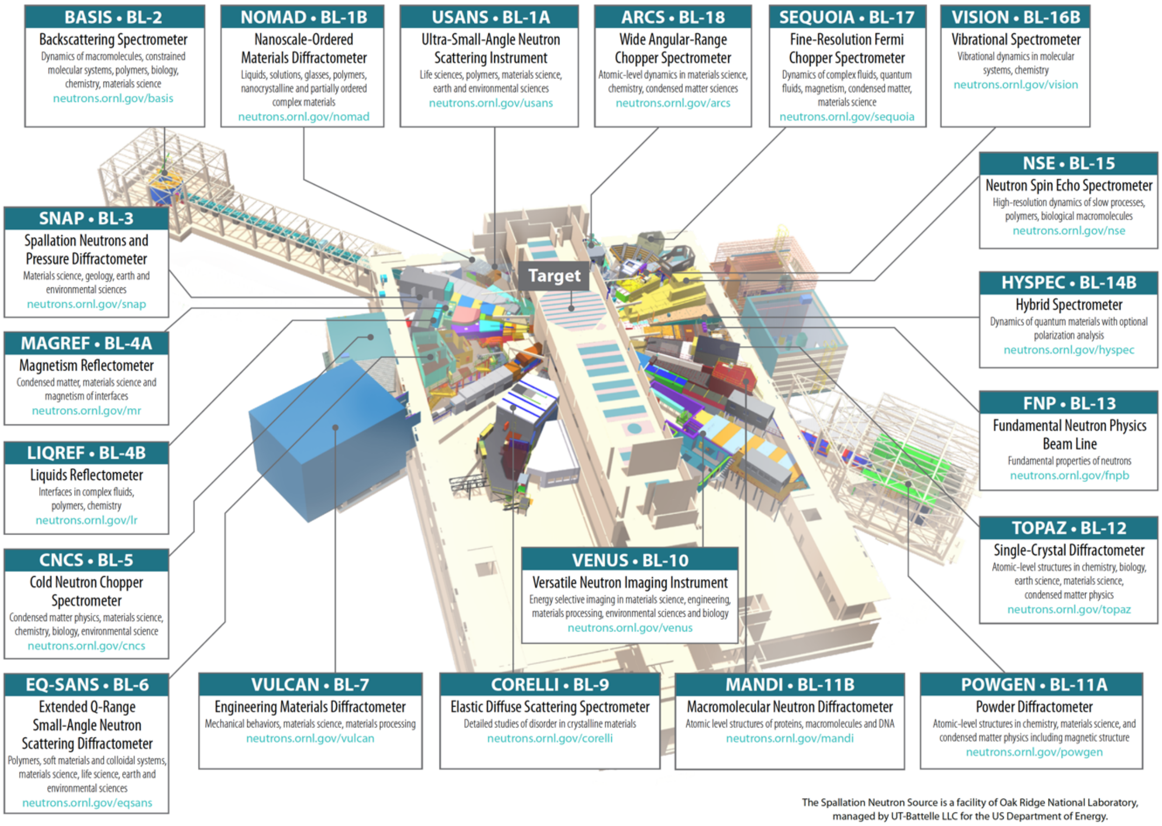


Figure 2. Layout of the SNS Instrument Suite as of August 2024.

Direct-Geometry Spectroscopy

Direct-geometry spectrometers have transformed the field of inelastic neutron scattering, enabling mapping of large volumes of data in 4D (**Q**, ω) space. SNS is home to four world-leading direct-geometry instruments. Of these four instruments, ARCS (BL-18) and SEQUOIA (BL-17) are thermal neutron spectrometers, whereas CNCS (BL-5) and HYSPEC (BL-14B) use cold neutrons. HYSPEC provides unique capabilities for polarized direct-geometry spectroscopy. These instruments are ideal for performing comprehensive inelastic neutron scattering exploration of lattice vibrations and magnetic excitations in a wide range of materials under a variety of sample environment conditions.

ARCS (BL-18)

ARCS is optimized to provide a high thermal neutron flux at the sample and a large solid angle of detector coverage. The spectrometer can select a wide range of incident energies, making it useful for studies of excitations from a few to several hundred millielectronvolts. Compared with SEQUOIA, the ARCS sample-to-detector distance is shorter, resulting in moderate energy transfer and wavevector resolution but increased angular detector coverage and consequently increased range of wavevectors.

SEQUOIA (BL-17)

SEQUOIA is the complementary thermal neutron direct geometry spectrometer. Compared with ARCS, SEQUOIA's longer final flight path results in fine energy transfer and wavevector resolution. The range of incident energies is similar for ARCS and SEQUOIA.

CNCS (BL-5)

CNCS is a high-resolution cold neutron direct-geometry spectrometer with strong performance at low incident energies (2 to 50 meV). Experiments at CNCS typically use energy resolutions between 10 and 500 µeV. A broad variety of scientific problems, ranging from complex and quantum fluids to magnetism and chemical spectroscopy, are being addressed by experiments at CNCS.

HYSPEC (BL-14B)

HYSPEC is a cold neutron direct-geometry spectrometer that incorporates Bragg focusing optics, making it well suited for measurement of excitations in small single-crystal specimens in a wide range of ancillary sample environments with moderate energy resolution. The Bragg optics enable monochromatic incident beams of both polarized (3.8 meV < E_i < 25 meV) and unpolarized (3.8 meV < E_i < 60 meV) neutrons. Combining the incident Bragg optics with a supermirror wide-angle polarization analyzer after the sample allows HYSPEC to perform full or partial neutron polarization analysis to provide unambiguous separation of nuclear and magnetic scattering.

Chemical Spectroscopy

BASIS (BL-2)

BASIS is a near-backscattering silicon crystal analyzer indirect-geometry time-of-flight spectrometer optimized for a very high energy resolution (currently 0.0034 meV full width at half maximum [FWHM]). The overwhelming majority of experiments at BASIS measure quasielastic neutron scattering in a broad array of systems from chemical, biological, and soft matter sciences that exhibit diffusional or relaxational dynamics on pico- to nanosecond timescales. A small minority of experiments at BASIS may be concerned with high-resolution inelastic scattering, such as rotational quantum tunneling of protons in methyl groups.

SNS-NSE (BL-15)

SNS-NSE is an ultrahigh-resolution neutron spectrometer for characterizing slow dynamics. SNS-NSE is a time-of-flight instrument: the Larmor precession of the neutrons spin in a preparation zone with magnetic field before the sample encodes the individual velocities of the incoming neutrons into precession angles. A symmetric decoding zone after the sample compensates for the precession angle accumulated and leads to the restoration of polarization by spin re-phasing, the so-called spin echo. If the sample changes the neutron velocity by a small amount (as low as 10^{-4}), then a loss of polarization is measured. The SNS-NSE is designed with superconducting technology with high magnetic field homogeneity and takes full advantage of state-of-the-art field correction elements, novel polarizing benders, and magnetic shielding for a reliable and precise operation.

VISION (BL-16B)

VISION is graphite crystal analyzer indirect-geometry time-of-flight spectrometer used for neutron vibrational spectroscopy. The science addressed by VISION is very diverse. Some commonly pursued topics include aqueous systems, hydrogen storage, organic chemistry, catalysis and surface chemistry, polymers, batteries and fuel cells, porous materials, minerals, complex hydrides, and proton conductors. Although measurements of “fingerprint” intramolecular excitations are most common at VISION, the spectrometer’s excellent energy resolution near the elastic line (~0.120 meV FWHM) and high neutron flux allow efficient probing of the density of states in both hydrogen-containing and non-hydrogen-containing systems.

Powder Diffraction

NOMAD (BL-1B)

NOMAD is a highly productive beamline; it is currently the fastest neutron diffractometer in the world. The high flux and medium resolution, combined with a large bandwidth of neutron energies and extensive detector coverage, allow NOMAD to carry out structural determinations of local order in crystalline and amorphous materials. The science performed on NOMAD is incredibly diverse, including liquids, solutions, glasses, polymers, nanocrystalline materials, and long-range ordered crystals.

SNAP (BL-3)

The SNAP diffractometer is a high-flux, medium-resolution instrument, using highly integrated advanced area detectors, beam-focusing optics, and a suite of pressure devices to study a variety of powdered, single-crystal, and amorphous materials under extreme pressure at temperatures ranging from cryogenic to high temperatures. Traditional Paris-Edinburgh presses are used to attain 25 GPa. The instrument staff and the instrument development team are making progress with large-volume diamond anvil cells in hopes of significantly extending the pressure range currently accessible to neutron diffraction. The goal is to routinely achieve pressures of 50 to 100 GPa for samples on the order of 0.05 mm^3. SNAP leads the world in the development of a novel diamond anvil cell compatible with neutron diffraction and, to the best of our knowledge, is the only facility that makes this capability available to the user program.

VULCAN (BL-7)

VULCAN is designed for studies of deformation, phase transformation, residual stress, texture, and microstructure. Load frames, furnaces, battery chargers, and other auxiliary equipment for in situ and time-resolved measurements are integrated into the instrument. As a time-of-flight diffractometer at the world's most intense pulsed, accelerator-based neutron source, VULCAN provides rapid volumetric mapping with a sampling volume of 2–600 mm^3 and a measurement time of minutes for common engineering materials. In extreme cases, VULCAN can be used to study kinetic behaviors in subsecond timeframes.

POWGEN (BL-11A)

POWGEN is a high-throughput, high-resolution neutron powder diffractometer that enables characterization of the crystal, magnetic, and local structure of novel polycrystalline materials. Scientific studies at this instrument encompass a wide range of novel materials, including energy storage materials, ceramic membranes for solid oxide fuel cells and oxygen sensors, hydrogen storage materials, high-entropy alloys, and thermoelectric materials. Fast data collection allows looking at in situ processes (e.g. solid-state synthesis, redox reactions and gas-solid interactions). Long *d*-spacing coverage enables the study of magnetic materials such as magnetic semimetals, multiferroics, high-T_c superconductors, charge and orbital ordering transitions, magnetocaloric materials, and molecular magnets.

Single-Crystal Diffraction

CORELLI (BL-9)

CORELLI (elastic diffuse scattering spectrometer) is optimized for studying the complex magnetic and structural disorder in single-crystal materials. The instrument is designed for scattering studies with a large momentum transfer range ($0.5 < Q < 16$ Å^{-1}) and appropriate energy resolution ($\Delta E \approx 0.89$ meV FWHM at $E_i = 25$ meV). The combination of quasi-Laue and cross-correlation techniques allows accurate mapping of elastic scattering signals over a broad range of reciprocal space at an unprecedented rate. The instrument is capable of hosting 91 detector modules, and 75 modules have been installed to date.

MaNDi (BL-11B)

MaNDi provides a powerful tool for determining the position of hydrogen atoms and orientation of water molecules as well as for identifying different chemical species in protein structures. The wavelength bandwidth is $\Delta\lambda = 2.15$ or 4.3 Å, which can be selected anywhere between 1 and 10 Å. Data can be collected on samples of 0.1 mm^3 or larger with unit cells in the range of 30–300 Å on edge. An experimental temperature range of 60 to 400 K is provided by an Oxford diffraction cryostream. MaNDi has a nearly its full complement of state-of-the-art Anger camera detectors. The instrument benefits from having samples with total replacement of hydrogen by deuterium (per deuteration) and the increased operating power of the accelerator. Recently, MaNDi has been prominently used for structural studies of coronavirus proteins that have been expressed, purified, and crystallized at ORNL.

TOPAZ (BL-12)

TOPAZ is a high-resolution time-of-flight single-crystal diffractometer for small-molecule and chemical crystallography. It uses a neutron wavelength-resolved Laue technique for data collection up to 0.25 Å in d_{min} or 25 Å^{-1} in Q_{max}. TOPAZ is capable of continuous 3D Q space mapping of specific regions of reciprocal space from a stationary single-crystal sample. This capability is desired for phase transition studies and diffuse scattering of either nuclear or magnetic origin. TOPAZ is gradually realizing its full potential for these science capabilities, despite the incomplete detector coverage (see the TOPAZ Detector Build-Out upgrade description). Future plans include a polarized beam option using an in situ pumped ^{3}He neutron spin filter system.

Small-Angle Neutron Scattering

USANS (BL-1A)

USANS is an ultrasmall-angle neutron scattering instrument dedicated to the study of structures at mesoscale levels. Its main science areas are geoscience, materials science, biology, nanotechnology, and environmental science. The instrument design is an advanced version of the classical Bonse–Hart double-crystal diffractometer adapted to the pulsed nature of SNS. Its accessible wavelength spectrum is provided by four Bragg reflections at 3.6, 1.8, 1.2 and 0.9 Å. The available Q range of USANS is 1×10^{-5} Å^{-1} < Q < 3×10^{-3} Å^{-1}, ideally complementing the small-angle neutron scattering (SANS) instruments at ORNL.

EQ-SANS (BL-6)

EQ-SANS is a time-of-flight small-angle neutron scattering diffractometer designed to study noncrystalline, nano-sized materials. It offers a broad dynamic Q range, and overall wide Q coverage from 0.002 Å^{-1} up to a uniquely high several inverse angstroms. The most frequently used 60 Hz operation mode offers a 3–4.3 Å wavelength band, and the 30 Hz mode offers two wavelength bands and a wider dynamic Q range. The instrument offers a range of sample environments such as Peltier-based linear sample changer, multiposition furnace, and rheometer or tensile stage, and it is presently being upgraded to accommodate a robotic sample changer.

Reflectometry

Neutron reflectometry probes surface and interfacial structures of thin films on length scales of 0.5 nm to 350 nm. Like other elastic neutron scattering and diffraction methods, the technique is sensitive to spatial variation in nuclear composition and magnetization.

MAGREF (BL-4A)

MAGREF provides the user community with capabilities to characterize nonuniform distributions of magnetization in nanoscale and mesoscale materials related to quantum condensed matter in different environmental conditions. The instrument provides polarized neutron beams, enabling measurements of specular and off-specular reflection and grazing-incidence small-angle scattering (GISANS) from vertical solid or solid/liquid interfaces. Polarized neutron beams are produced by reflection or transmission polarizers. Polarization analysis of the scattered beams with a mirror analyzer or ^{3}He filter is optionally available. MAGREF is primarily focused on studies of materials with a net magnetization—magnetization that can be perturbed by many environmental variables, including magnetic and electric fields, temperature, pressure, stress, and light. Polarized neutron beams also enable some studies of nonmagnetic materials such as soft matter; for example, by quantifying incoherent scattering, or phase-inversion using the magnetic reference layer technique.

LIQREF (BL-4B)

LIQREF measures specular and off-specular neutron reflectivity in a horizontal sample geometry from solid surfaces, tilted solid/liquid interfaces, and free liquid surfaces. The neutron probe wavelength and flux require samples no smaller than about 1 × 1 cm^2 deposited on atomically smooth and centimeter-scale flat substrates such as silicon, quartz, sapphire, or water. The most commonly used substrate is a Ø50 mm, 5 mm thick silicon wafer. A variety of sample environments are supported, including an 18-slot robotic sample changer, temperature-controlled liquid/solid and potentiostatically controlled electrochemical cells, vacuum and gas-handling chambers, a rheometer, and a Langmuir trough.

Neutron Imaging

VENUS (BL-10)

The VENUS instrument recently completed construction and is currently in commissioning. VENUS will be one of the most advanced beamlines for neutron imaging, providing US researchers with exciting new ways of studying a diverse range of materials. Neutron imaging is a powerful technique used to generate pictures of the internal structure of materials. The images, called radiographs, are similar to clinical x-rays that use contrast variations to reveal the internal structure of objects as neutrons are absorbed or deflected by different atoms inside a material. Whereas the MARS imaging beamline at HFIR utilizes a steady-state or constant beam of neutrons, VENUS will feature time-of-flight capabilities enabled by the pulsed nature of SNS. Leveraging time-of-flight, VENUS combines the properties of transmission and sensitivity to elements and crystalline structures that will allow users to collect data on both the structure and behavioral dynamics of materials at the atomic scale.

Current HFIR Instrument Suite

Figure 3 shows a layout of HFIR instrument which are described below, grouped by instrument suite.

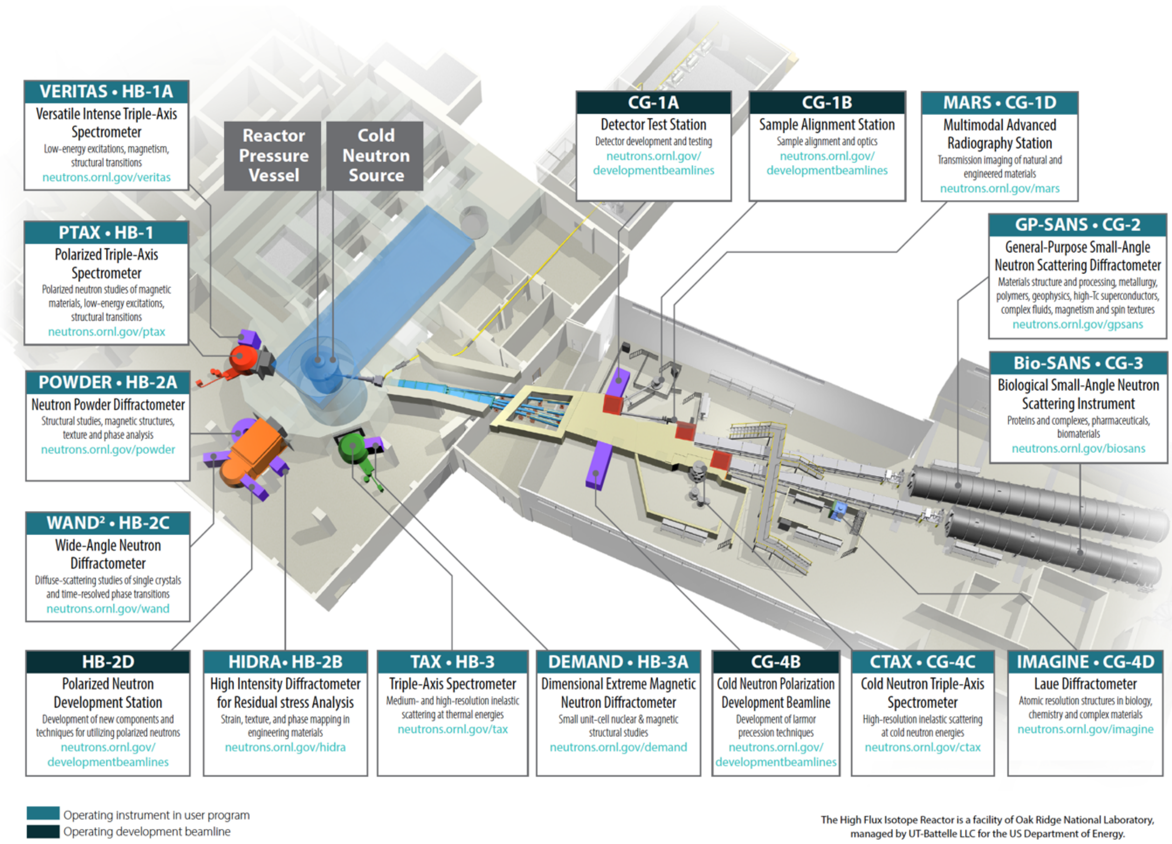


Figure 3. Layout of the HFIR Instrument Suite as of August 2024.

Triple-Axis Spectroscopy

Triple-axis spectrometers are highly flexible instruments designed for high-flux measurements in a limited range of wavevector–energy space. The HFIR triple-axis spectroscopy instrument suite includes three thermal neutron triple-axis spectrometers (HB-1A, HB-1, and HB-3) and a cold neutron triple-axis spectrometer (CG-4C). HB-1 is specifically designed for measurements with full neutron polarization analysis. All four triple-axis spectrometers are ideally suited to parametric studies and support a wide range of sample environment equipment. They complement the suite of direct-geometry spectrometers at SNS with their ability of mapping out small volumes of **Q** and ω space quickly and efficiently under extreme sample environment conditions.

VERITAS (HB-1A)

VERITAS is a fixed incident energy triple-axis spectrometer. It employs a double-bounce pyrolytic graphite monochromator assembly and a pyrolytic graphite analyzer to produce an intense, clean beam at λ = 2.38 Å with low background and an excellent signal-to-noise ratio. HB-1A is mostly used for elastic scattering studies of small crystals and thin-film samples with weak magnetic scattering signals, complementing the suite of diffractometers at HFIR and SNS.

PTAX (HB-1)

HB-1 is a polarized triple-axis spectrometer with full neutron polarization analysis capability. Currently at HB-1 the neutron beam is polarized using a fixed vertically focused Heusler monochromator and a flat Heusler analyzer, which will be replaced with high-quality Heusler monochromator and analyzer system directly acquired from Laboratoire Léon Brillouin (Saclay, France) in the near future. Several unique capabilities are also available at HB-1, including the high-resolution Larmor diffraction and spin-echo capability utilizing Wollaston prisms, and a spherical neutron polarimetry capability.

TAX (HB-3)

HB-3 is as a versatile triple-axis spectrometer with very high incident beam flux. The monochromator system at HB-3 has three variable vertical-focus monochromators—pyrolytic graphite (PG) (002), beryllium (002), and pressed silicon (111)—allowing for selection of incident energies up to 180 meV., PG (002) provides high flux, beryllium (002) provides better energy resolution at higher energy transfers, and silicon (111) provides a clean beam with no $\lambda/2$ contamination. The availability of these three monochromator crystal choices makes this spectrometer extremely versatile for a wide range of studies.

CTAX (CG-4C)

CTAX is a cold neutron triple-axis spectrometer with variable incident energy (2–18 meV) and sample–analyzer distances. The PG (002) monochromator is vertically focused, and the PG (002) analyzer has a fixed vertical focus and variable horizontal focus. CTAX enables analysis of low-energy excitations with high signal-to-noise.

Powder Diffraction

POWDER (HB-2A)

POWDER is a workhorse instrument for magnetic and crystal structural studies of powder samples as a function of intensive conditions. The low angular coverage and clean background makes POWDER ideal for studying new, complex, magnetically ordered systems. At present, POWDER is the only beamline in the powder suite to utilize polarized neutrons, necessary to determine local anisotropy and weak ferro-/ferrimagnetism.

WAND^2 (HB-2C)

WAND^2 is a versatile instrument designed to provide fast measurements of medium-resolution powder diffraction data and measurements of small signals or diffuse scattering in single crystals. The 2D position-sensitive neutron detector with out-of-plane coverage enables measurements of a large volume of reciprocal space, necessary to identify magnetic propagation vectors and study diffuse scattering. The high flux of WAND^2 allows for fast data sampling, ideal for parametric and kinetic studies of powders.

Single-Crystal Diffraction

DEMAND (HB-3A)

DEMAND continues to play the principal role of determining the magnetic and crystal structures of the small unit cell system (cell volume <10^5 Å^3). Unpolarized and polarized neutrons are both available and easily switchable. Currently, DEMAND runs with one column of solid-state Anger camera detectors, which covers 16° in horizontal and 48° in vertical directions. Ongoing upgrade plans include expanding the detector coverage by adding two additional columns of magnetic field insensitive detector modules, relocating the sample table farther downstream by 2 m, and purchasing a dry high-T_c superconducting magnet.

IMAGINE (CG-4D)

IMAGINE has the potential to have broad scientific impact and a diverse user community for the analysis of light atom positions in materials that are of interest across the fields of structural biology, pharmacology, chemistry, condensed matter physics, nano-structured materials, and geological sciences. The IMAGINE neutron image plate diffractometer is designed for rapid collection of high-resolution (~1.1 Å) Laue or quasi-Laue data from small single crystals (>0.1 mm^3) of moderate unit cell size (~100 Å), primarily for structural biology. The instrument uses variable short- and long-wavelength cutoff optics to provide multiple wavelength configurations, and a pair of elliptical focusing mirrors delivers 3 x 10^7n

$s^{-1}cm^{-2}$ into a 3.5 × 2.0 mm^2 focal spot at the sample position (dλ/λ ≈ 25%). IMAGINE has been hosting the development work on polarizing the sample nuclei to enhance the scattering power of hydrogen, thus avoiding the laborious efforts required to deuterate samples. The IMAGINE instrument will be relocated to a better optimized guide during the next HFIR Beryllium Reflector Replacement (HBRR), and the flux on sample is expected to double.

Residual Stress Analysis

HIDRA (HB-2B)

HIDRA is a world-class, high-flux, engineering diffractometer ideal for spatial characterization of microstructures in large-scale engineering components. The instrument is flexible, meaning the instrument configuration is defined by the sample material and geometry. The instrument is focused on applied and industrial materials engineering problems. It has also supported new science needs arising from additive manufacturing. HIDRA fills a unique niche to nondestructively map large-scale engineering components using diffraction. Information obtained from diffraction can take the form of residual stress/strain, phase, and crystallographic texture. Applications for mapping include materials joining (e.g., welding, brazing, friction stir welding, and riveting), heat-treated samples, forgings, extrusions, bearings and races, fasteners, components for transportation and aerospace, pressure vessels and piping, nuclear engineering components, and increasing parts made through additive manufacturing (AM) of metal components. Mapping of full-strain tensors for residual shear strain maps is crucial in advanced manufacturing processes such as fusion powder bed AM, direct energy deposition, and additive friction stir deposition.

Small-Angle Neutron Scattering

GP-SANS (CG-2)

GP-SANS is a general-purpose small-angle neutron scattering diffractometer designed to probe structural features in a wide variety of systems such as metallic alloys, ceramics, catalysts and adsorbents, superconductors and other correlated electron materials exhibiting long-range order, geological systems, biological systems, colloids and complex fluids, and polymers. This instrument's open-space sample area can accommodate a wide variety of sample environments, including a robotic sample changer. It offers a wide Q coverage (0.0007–1.3 $Å^{-1}$) and the highest flux on sample among the SANS instruments at ORNL. The accessible wavelength band is 4–25 Å, with a relative triangular width of 0.09–0.45 Δλ/λ.

Bio-SANS (CG-3)

The Bio-SANS) instrument operates as part of the Center for Structural Molecular Biology and is dedicated to analyzing complex biological systems. It features a combination of wing, mid-range, and main detector arrays. This three-detector system enhances data quality, reduces Q resolution mismatch, increases detector coverage, and enables subminute time resolution, benefiting hierarchical systems analysis. The instrument also features a simplified measurement setup and execution for users by alleviating the need for users to know instrument-specific details. A set of rapid measurements is enabled by a Robotic Sample Changer. Bio-SANS uses a wavelength range of 6–25 Å, has variable-wavelength resolution of 9%–45%, and an accessible Q range of 0.0009–1 $Å^{-1}$.

Neutron Radiography

MARS (CG-1D)

The MARS instrument provides radiography and computed tomography imaging capabilities for applications in AM, materials science, geoscience, biology, energy, and transportation. MARS uses a polychromatic neutron beam in the cold range for neutron imaging measurements. Apertures (with different diameters D, pinhole geometry) are used at the entrance of the helium-filled flight tube to allow variations of the figure of merit L/D, where L is the distance between the aperture and the detector where the image is produced. The value of *L*/*D* can vary from 400 to 2000. Samples sit on a translation/rotation stage for alignment and tomography purposes. Its maximum field of view is 86 mm × 86 mm. Also available are ^{6}LiF/ZnS scintillators varying from 50–200 µm.

Development Beamlines

Detector Test Station (CG-1A)

The CG-1A instrument uses a 4.2 Å monochromatic beam from a PG (002) monochromator for equipment testing and development. The variable divergence and reasonably high neutron flux enable the detector group and external user groups to characterize their prototypes for spatial resolution and rate capability; detectors ready for deployment also undergo final performance evaluation at the beamline. Recent efforts include calibration of Anger cameras for diffraction beamlines, testing of the new dome Anger camera prototype assembly, characterization of new scintillators, and preparation of TimePix-based microchannel plate detectors for neutron imaging. The Neutron Optics and Polarization group uses the beam occasionally for the characterization of various components. Currently the beamline is being equipped to host supermirror reflectivity measurements and data acquisition software development.

HB-2D

HB-2D will provide the neutron scattering community with a dedicated multipurpose platform for the R&D of advanced neutron scattering techniques and components, essential to ensure ORNL's leadership in neutron instrumentation. The scope of HB-2D will include the R&D of polarized neutron instrumentation and methodology, ^{3}He neutron spin filters, neutron spin manipulation devices, advanced neutron optics, and detectors. The instrument will use a silicon (220) monochromator to produce a 2.43 Å thermal beam for polarized neutron studies. An additional monochromator will deflect the half wavelength of 1.21 Å to a detector test station.

CG-4B

The CG-4B instrument uses a 5.5 Å monochromatic beam off a silicon monochromator for the development of cold neutron polarization technologies for spherical neutron polarimetry, RF spin flippers, and, more generally, Larmor precession optics. The beamline is also used for feasibility tests of polarized SANS applications.

Crystal Alignment (CG-1B)

The CG-1B instrument is a two-axis diffractometer with a single detector principally used to align single crystals for follow-up experiments at either HFIR or SNS. This capability ensures users are ready for these experiments and improves the overall efficiency of the user program. The alignment instrument is also well suited to testing and aligning monochromator crystals for new or upgraded instruments.

Prioritization Processes

This section describes the processes used for prioritization of mid-scale investments, instrument improvement projects, and new instruments. Figure 4 illustrates how plans for upgrades, new capabilities, new sample environments, and new instruments are identified, developed, prioritized, and funded. Input is collected from various sources, including communication with our current users, user surveys and feedback received from the SNS–HFIR User Group, broader scientific trends, comparison of capabilities with those at other facilities, science review committee feedback, and the recommendations from periodic instrument suite assessments. Concepts for upgrades or new instruments based on this input are then championed by a principal investigator in the user community or a Neutron Sciences Directorate staff member, and a proposal is developed. Proposals for upgrades are solicited annually. These proposals fall into two categories: mid-scale investments or instrument improvement projects, depending on scope and resource requirements. The projects are part of our commitment to provide world-leading capabilities to the user community. They are typically funded from the Neutron Scattering Division (NSD) operating budget but may be funded from external sources. For new instruments, the investment requires external funding, possibly including funding from other US government sources (e.g., DOE, National Science Foundation (NSF), National Institutes of Health), funding from international agencies, or industry.

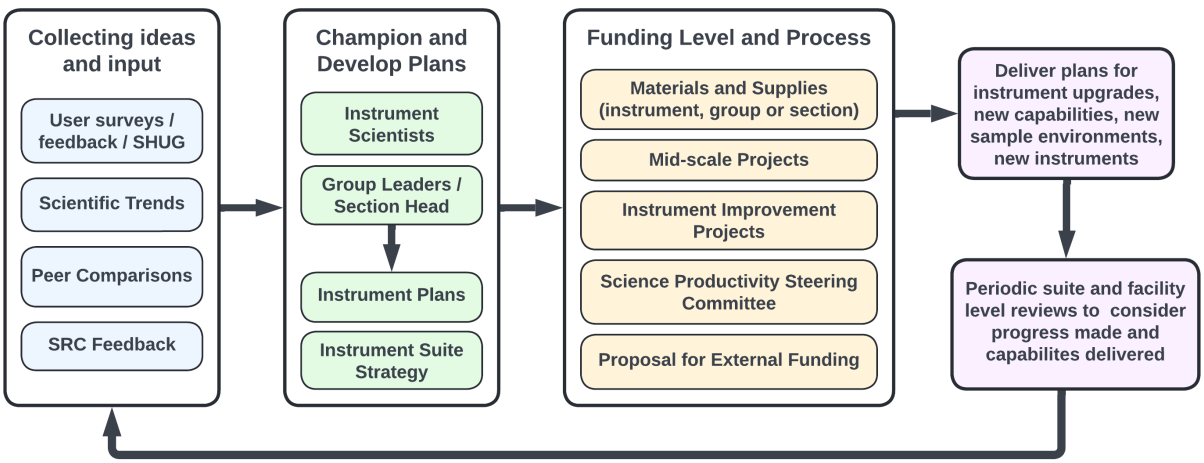


Figure 4. Process developing and prioritizing plans for instrument upgrades, new capabilities, new sample environments, and new instruments.

Mid-Scale Investments

Mid-scale investments have a total cost estimated to not exceed $500k and typically require minimal engineering effort. Many sample environment purchases, such as sample changers for increased automation, fall within this category. Proposals for mid-scale investments are reviewed and prioritized by the NSD director and section heads in consultation with sample environment steering committees and science initiative coordinators.

Instrument Improvement Projects

If the required funds exceed $500k or substantial staff resources are required, then items are classified as instrument improvement projects. The Science Productivity Steering Committee (SPSC), composed of NSD senior scientists and managers, is responsible for prioritizing new projects. The SPSC considers the scientific impact of new projects; reviews cost, resources, and schedule; and makes funding recommendations to the NSD director for projects to advance. An annual timeline for the instrument improvement project process is described in detail in Figure 5 and consists of an NSD call for proposals, initiation review, conceptual design review, final design review, and a project execution plan.

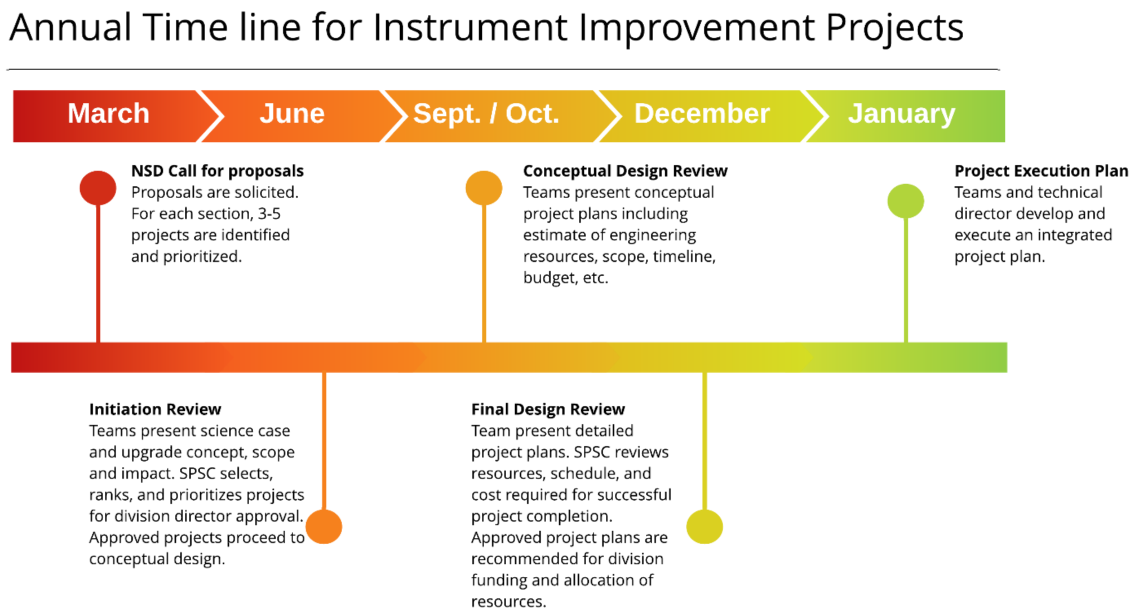


Figure 5. Annual timeline for review, prioritization, and approval of instrument improvement projects.

New Instrument Selection

A process has been developed for future instrument selection across SNS FTS, SNS STS, and HFIR. We are working with the community and the SNS–HFIR User Group to establish the mandates and composition of three expert committees: Science Advisory Committee, External Advisory Committee, and Internal Expert Committee. Their general functions are described below. The initial instruments selected as part of the STS project will follow a process defined by the project, but all subsequent STS instrument decisions will follow the process defined below.

Committees and Individuals Involved

- The associate laboratory director (ALD) for Neutron Sciences makes the final decisions.
- The directors of NSD, the Neutron Technology Division (NTD), and STS (while still a project) provide direct input to the ALD at decision points.
- An external Science Advisory Committee (SAC) should advise the ALD on whether the existing and proposed instruments represent a comprehensive set of capabilities that meet the needs of the scientific community. In response to the SAC's advice, the ALD may ask an internal or external group to consider proposing a needed instrument.
- An Internal Expert Committee (IEC), with representatives from NSD, NTD, and (while running) the STS project, will conduct an initial evaluation of a letter of intent or preliminary instrument proposal. The IEC members will be named by the Neutron Sciences ALD in consultation with the directors of NSD, NTD, and STS (while applicable). The IEC should meet regularly.
- An External Advisory Committee (EAC), composed of researchers from outside ORNL, should include a selection of experts on neutron scattering facilities, closely related techniques such as synchrotron radiation, and science covered by these facilities. The EAC will evaluate a more detailed proposal. The EAC members will be named by the Neutron Sciences ALD in consultation with the directors of NSD, NTD, and STS (while applicable).

- The Instrument Concept Team (ICT) is a group of researchers who wish to propose a new instrument to be built at HFIR, FTS, or STS

Brief Description of Instrument Selection Process

The process for the ICT has three possible stages, each of which can also be an entry point:

i. Letter of intent
ii. Preliminary proposal
iii. Full proposal.

The first two stages are evaluated by the IEC, which provides recommendations to the ALD, who will decide whether the instrument should proceed to the next stage. The third stage is evaluated by the EAC, which provides a recommendation to the ALD. The ALD makes final decisions.

Detailed Instrument Selection Process

The instrument selection process is illustrated in Figure 6 and is detailed below.

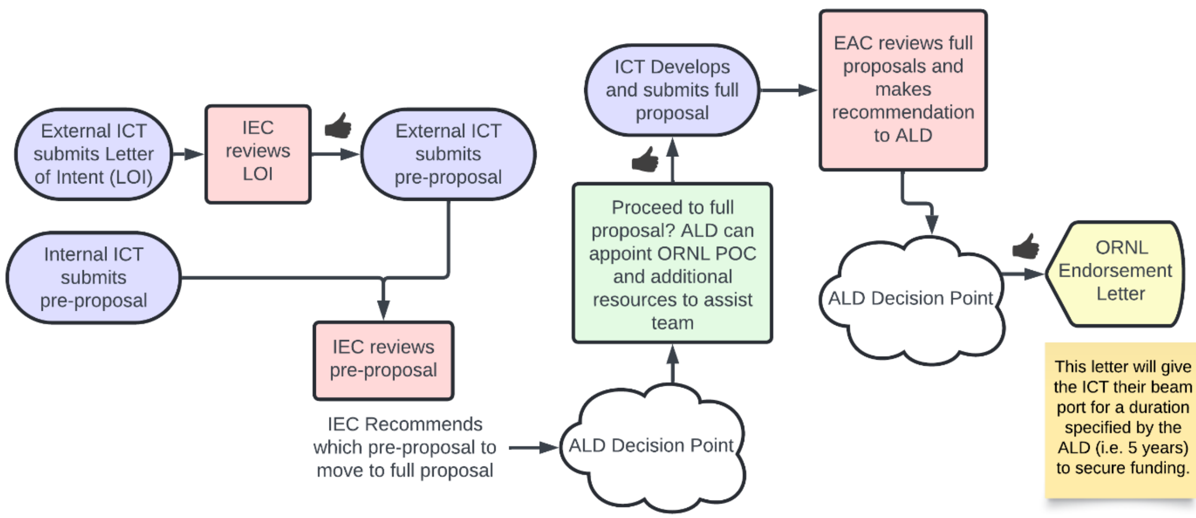


Figure 6. Process for selecting new instrument concepts. ALD = Associate Laboratory Director; ICT = Instrument Concept Team; IEC = Internal Expert Committee; EAC = External Advisory Committee.

1. An instrument concept is developed by a group (i.e., ICT) or individual inside or outside of ORNL. The ICT may submit a letter of intent, briefly describing the instrument and its intended applications, for a preliminary evaluation by the IEC. The IEC will consider whether the instrument concept is reasonable. If so, then the IEC can recommend proceeding to a preliminary proposal. The IEC should identify the best source for locating the instrument. If warranted, then the IEC may recommend to the ALD that the Neutron Sciences Directorate provide some resources to help the ICT develop the concept. This possibility is meant to encourage creative thinking by groups that may not already be heavily committed to neutron scattering.
2. The ICT produces a preliminary proposal. The preliminary proposal should address the following questions:
    - Science case: What is the purpose of and scientific motivation for this instrument? What is the justification for making the measurements with neutrons rather than x-rays or

some other probe? What is the user community for the instrument? Has the user community been consulted?

- Instrument description: What does one plan to build, and how does it fit in the context of existing instruments?
- Source: Is this instrument proposed for FTS, STS, or HFIR, and what moderator and/or beamline is requested? An explanation of the choice should be included.
- Funding: Does the proposing group plan to seek full or partial funding from a funding agency? If so, which agency? Why do the proposers believe the agency will be interested in supporting this instrument?

3. The preliminary proposal is evaluated by the IEC. The IEC will consider the feasibility and sensibility of the preliminary proposal and will recommend whether the proposing group should be invited to prepare a more detailed full proposal. The IEC should provide some guidance to the proposing team if the more detailed proposal needs additional technical information.
   - The IEC should meet quarterly whenever there is business to be done.
   - The IEC is free to seek additional advice from internal and/or external experts on technical or scientific matters that are relevant to the proposal.
   - The IEC will maintain a prioritized list of instrument concepts, and new concepts will be inserted into the list as appropriate.
4. The ALD will decide whether to accept the IEC recommendation in consultation with the directors of the NSD, NTD, and (while applicable) STS.
5. If the recommendation is positive, then the proposing group will be asked to prepare a more detailed full proposal with a preliminary cost estimate and technical details recommended by the IEC. At the discretion of the ALD, for proposals originating from external groups, an ORNL staff member (or members) may be made available to help with technical details. If allowable, then program development funds may be allocated to the exercise.
6. The proposing group will prepare the full proposal and present a briefing to the EAC.
   - Unsuccessful proposals from the first phase of proposed instruments for STS will begin at this stage if they are able to address the concerns of the STS Instrument Review Committee.
7. The EAC should meet at least annually, and when necessary, twice a year, to consider the briefings from proposing groups. The EAC will recommend a course of action to the ALD for each proposal.
   - Possible recommendations may include the following:
     i. Reject the instrument.
     ii. Table the instrument for reconsideration later and request more information.
     iii. Proceed to conceptual design with one of several subsequent aims:
        - Build within existing budget.
        - ORNL should apply to DOE to build as a project or part of a project.
        - External group should apply for funds from DOE, NSF, or another agency.
   - Detailed conceptual design should be performed by ORNL staff, with input from proposing groups.
   - Instruments chosen for decisions ii or iii above will be added to the prioritized list maintained by the IEC, with priority assigned by the ALD.
8. The ALD will make the final decision how to proceed. During the lifetime of the STS project, the STS project director will provide input to the decision for all instruments proposed for STS. For all instruments, additional input may be sought from the Neutron Advisory Board and relevant directors or staff. The full design will generally be part of the project once funded.

9. If the proposal is successful, then an ORNL endorsement letter will be sent to the ICT and will serve to reserve the beam location for this instrument for a specified period of time (e.g., 5 years) to allow the proposing group to secure funding.

Finally, we note that no policy is currently in place for retiring instruments, and such a policy will be developed. Regularly gathered information such as instrument peer comparisons, user feedback, and instrument suite assessments would be used to identify instruments that could potentially be retired. Although the policy remains to be developed, it will likely involve the SAC and/or the EAC.

SNS Instrument Suite

The current instrument suite at SNS provides world-class capabilities that were chosen and optimized in collaboration with the user community. The four empty beam ports at SNS present opportunities for new instruments. Additionally, consideration of optimizing the instrument suite between HFIR and SNS, and additional needs identified in collaboration with the user community lead to potential opportunities for instrument relocations. The overall roadmap for SNS is described in Figure 7, including options for empty beam ports and possible relocation and repurposing of beam ports. This roadmap is described in detail in this section.

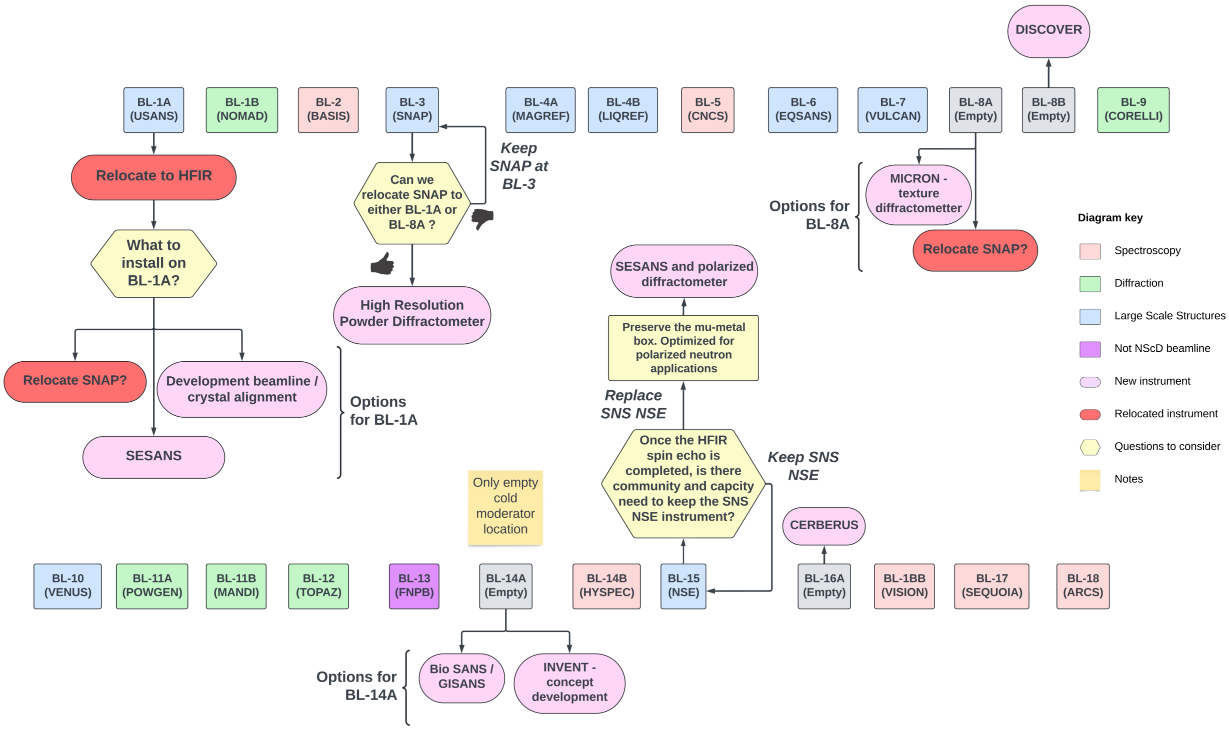


Figure 7. Diagram showing possibilities for future instruments at SNS together with possible instrument relocations.

The plans described here have been developed in consultation with the user community and have been considered by external review committees. The IAB convened in 2018 and produced a report that included the following recommendations for SNS:

- "The IAB recommends that ORNL add new instruments to the FTS."
- The following specific recommendations related to new instruments were made:
    - The time-of-flight imaging instrument VENUS was identified as the highest priority.
    - Adding capacity and capabilities for powder diffraction was also prioritized, and the IAB felt that "the two additional powder diffractometers, DISCOVER and HiResPD, should also be built at FTS with high priority." The IAB recognized that HiResPD requires instrument relocation but felt this capability was of sufficient importance to consider this relocation.

Some other specific comments from the IAB that are relevant to the plans are described in the following subsections as appropriate. As the IAB report has strongly guided our plans at both HFIR and SNS, this report is included as an appendix to this document.

New Instrument Possibilities

Currently, SNS has four empty beam ports. This section discusses the parameters of these beam ports and other factors that limit the possible deployable instruments. Potential concepts consistent with the moderator-viewed and physical constraints and that provide impactful capabilities to the user community are also discussed. The locations of these beam ports (BL-8A, BL-8B, BL-14A, and BL-16A) are shown in Figure 8, and Table 4 lists the moderator types and characteristics of these ports.

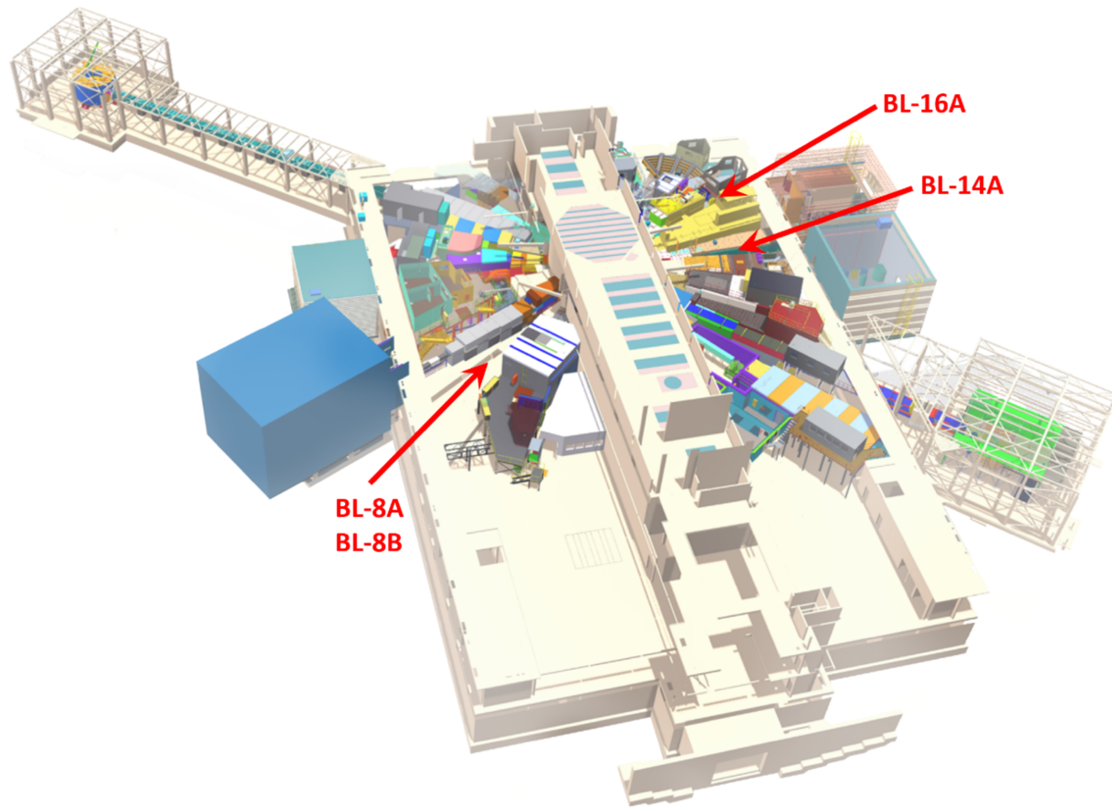


Figure 8. Instrument layout at SNS with the 4 empty beam port locations identified.

Table 4. Description of the four empty beam ports at SNS.

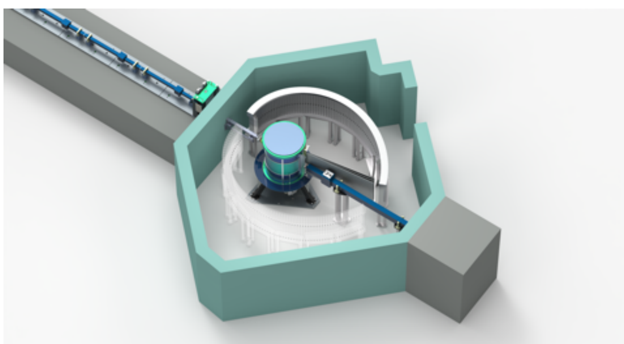
Beamline	Moderator type	Beam characteristics
8A	Shallow-poisoned, decoupled, ambient H_2O	Sharp pulses of thermal neutrons; high λ-resolution
8B	Shallow-poisoned, decoupled, ambient H_2O	Sharp pulses of thermal neutrons; high λ-resolution
14A	Coupled, cold para-H_2	Broad pulses of cold neutrons; high flux
16A	Deep-poisoned, ambient H_2O	Broad pulses of thermal neutrons; high flux

Ideal instrument types are driven by the moderator parameters. The two ports on BL-8 are best suited to hosting thermal neutron diffractometers, BL-16A is well suited to a thermal neutron spectrometer, and BL-14A is the most versatile and could host multiple instruments, including SANS, diffraction, and spectroscopy. The shared nature of these beam ports imposes restrictions on what is possible. BL-14A is a shared beam with HYSPEC (BL-14B), and BL-16A is a shared beam with VISION (BL-16B). BL-8 has the most flexibility because neither port is occupied. However, as described in the following subsections, DISCOVER is our highest priority on BL-8B, and this decision imposes constraints on what is possible on BL-8A. The concepts listed here are driven not only by scientific community needs but also by careful consideration of the space available to build an instrument. These details are described below in the following subsections.

BL-8

Of the empty ports, BL-8 provides the best opportunity for optimization because neither of the shared ports (8A/8B) are currently occupied. Potential instruments on these ports will be complementary to STS because they view a high-resolution ambient water moderator. The ports are well suited to thermal neutron diffractometers. The DISCOVER instrument concept is quite mature and has been socialized with the user community and considered by powder diffraction suite reviews. With DISCOVER on BL-8B, options are available for BL-8A, but the geometry is constrained, so those options are limited. One option for BL-8A is the MICRO concept designed to provide neutron texture mapping capabilities currently not available to the US user community. These two instrument concepts are described below.

DISCOVER (BL-8B)



DISCOVER (illustrated at left) will supply the scientific community with a platform for front-line investigations of the delicate interplay of global and local atomic symmetry, for examination of how order evolves from the atomic to macroscale, and for discovery of how these features respond to external perturbation to deliver new functionality. This instrument will fill critical capability gaps for the exploration of synthesis science, energy storage technology, quantum materials, mechanical characteristics, and catalysis and sorption processes. Key scientific opportunities include expanding the possible materials and structures that can be made; creating new design rules for development of new energy storage technologies; advancing enhanced materials classes for chemical separations, conversion, and utilization; and ushering in new paradigms for controlling emergent states of matter. Day one experiments will allow the community to answer urgent questions: *What causes the formation of undesired amorphous phases and nanodomains in solid state cathode materials of rechargeable batteries, and can they be avoided? How does water interact with carbide and carbon supported catalyst surfaces, and how does this limit performance? How can chemical short-range order and associated local lattice distortions provide next generation alloys additional strength and stability?* And *what chemistries, porosities, and defects enable self-healing and regeneration under real working conditions?*

Key Science Areas

1. Reaction pathways and mechanisms
2. Materials for energy storage and conversion
3. Sorbent and catalyst performance
4. Quantum materials

5. Mechanical characteristics

DISCOVER will provide detailed mechanistic insight into structural rearrangements while materials are in use, or being created, with simultaneous diffraction (for crystalline phases) and high-fidelity PDF (for liquid, amorphous, and nanostructured/disordered phases), also providing information about the nature and chronology of any intermediate-range structural order as phases form.

A rich history of community support and engagement led to the DISCOVER beamline concept. At the user workshop, "Delivering on the Promise of Powder Diffraction" in June 2013, 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. A few years later, the Powder Diffraction Working Group at the STS Workshop held in October 2015 named the instrument concept as its top priority for FTS. The inaugural powder diffraction suite assessment concluded as a leading statement in their executive summary:

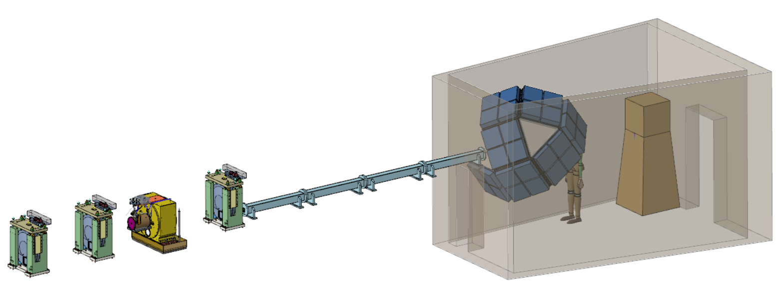
> *Our strong recommendation is to construct a rapid acquisition but medium-resolution quiet and stable diffractometer at BL-8 on the FTS as quickly as possible ... Such an instrument will restore the US lead in PDF studies of nanostructure, while filling an important gap in our capabilities for in-situ/in-operando studies and should be constructed with all haste.*

The DISCOVER Beamline Workshop (2017) was organized to define the goals, instrument concept, and design requirements for DISCOVER; review engineering and neutronics calculations; and outline a beamline concept. It was attended by an international committee of physics, chemistry, and materials experts as well as leaders in neutron diffraction and instrumentation. Since then, the DISCOVER beamline concept has been discussed at numerous conferences. In 2018, the beamline was endorsed as a top priority for FTS instruments by both the Materials Chemistry and Synthesis and Quantum Materials and Phenomena focus groups at the Neutron Users New Instrument Workshop. As described above, DISCOVER was also identified as a priority by the IAB.

The instrument concepts described herein for BL-8A, BL-16A, and BL-14A are preliminary concepts that are compatible with the restrictions imposed by the shared beam port. These concepts have not been prioritized and have had limited community engagement.

MICRON (BL-8A)

The short flight path (18 m) on a high-resolution, shallow-poisoned, decoupled ambient H_2O moderator on BL-18A is ideal to support MICRON: diffractometer for the **M**easurement of **I**n-situ **Cr**ystallographic **O**rientatio**n**. MICRON (illustrated at right) delivers one order of magnitude more neutron flux at its sample position compared with the previous, most advanced dedicated texture instrument in the United States. The designed *Q* range coverage from 1 to 24 $Å^{-1}$ enables measurements of full pole figures of a sample with minimal rotations. The open access from the instrument's tail end allows for movement of complex sample environment and a robotic arm sample changer for high versatility and throughput. MICRON is a cost-effective and easy-to-build instrument, and it will benefit from most available technologies for its detector and sample environments.



MICRON will be a unique tool to investigate microstructure and phase transformation of materials for structure–property relationships by taking advantage of the high-flux and high-resolution characteristics of BL-8A. 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. This would lead to thorough understanding of material properties optimization during materials processing. The high flux allows small samples or even thin samples—which often possess strong texture-correlated materials properties—to be investigated in situ by MICRON.

Key Science Areas

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 pathway, 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 allows for the necessary understanding to control preferred orientation to improve physical properties.

CERBERUS (BL-16A)

Of the remaining beam ports at SNS, BL-16A is one of the most restricted in terms of space because of interference between SNS-NSE (BL-15) and VISION (BL-16B). An instrument concept named CERBERUS,[1] shown in Figure 9, has been optimized for this space and will provide three distinct capabilities:

1. An alignment station to perform single-crystal alignments for samples to be later used on SNS and/or HFIR spectroscopy experiments. This capability will lead to more successful experiments at both facilities and improve overall efficiency.
2. A beryllium-filter analyzer indirect-geometry spectrometer optimized for near-infrared (>100 meV) spectroscopy. This capability will serve as an excellent complement to VISION, where the much finer energy resolution reduces intensity at higher energy transfers. Scientific areas that can benefit from improved performance at high energies include catalysis, in which many catalytic reactions involve making and breaking C–H bonds, which have stretching frequencies around 3000 cm^{-1}, and studies of oxide surfaces, which have O–H stretching modes around 3500 cm^{-1}.
3. A high-throughput nuclear cross-section measurement station. This capability can provide valuable experimental verification of cross sections needed in codes such as SCALE (a comprehensive modeling and simulation suite for nuclear safety analysis and design developed and maintained by ORNL) and Monte Carlo N-Particle (a general Monte Carlo code for neutron and photon transport developed by Los Alamos National Laboratory).

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[1] Matthew Frost, Jesse Brown, Franz Gallmeier, Ovidiu Garlea, Klaus Guber, Timmy Ramierz-Cuesta, and Kyle Schmmitt, *CERBERUS: A Multi-Purpose Spectrometer and Alignment Station at SNS*. ORNL/TM-2023/2823 (2023).

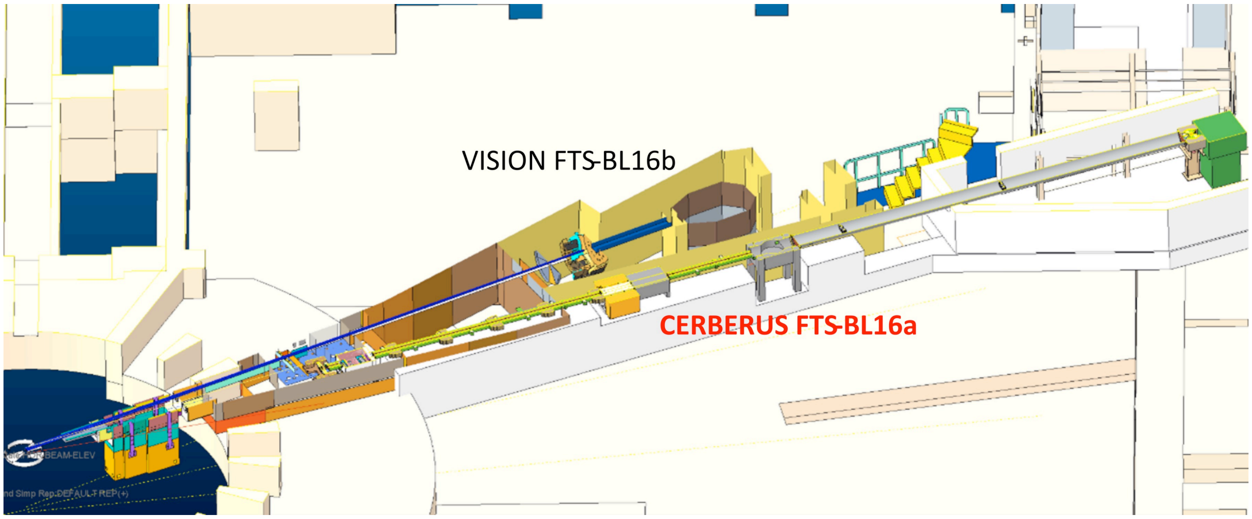

Figure 9. The CERBERUS concept on BL-16A shown next to VISION (BL-16B).

These three experimental applications would require no substantial technical developments, are complementary in their technical requirements, and provide capabilities that serve multiple missions.

The beryllium-filter spectrometer component of this concept was previously called BeFAST. This concept was presented as part of both chemical spectroscopy suite assessments and was endorsed by these committees. The IAB recognized the value of this instrument but said, “it would extend capabilities for chemical spectroscopy but is not an urgent short-term need.” This feedback lowered the priority of BeFAST and led to consideration of an expanded scientific scope as described above.

BL-14A

The most important motivation for placing a SANS instrument at BL-14A is to increase availability for this technique. Currently, very few SANS instruments are available for the US research community. The three SANS instruments at ORNL are highly oversubscribed, as were the instruments at NCNR while it was in operation. The lack of availability of beam time is limiting the development of the user community and is impeding the growth of important scientific fields, specifically soft condensed matter. SNS presently hosts only one SANS instrument. Of the available beam ports, only BL-14A views a coupled, cold hydrogen moderator, which is ideal for SANS because it provides long-wavelength neutrons—needed for probing large-scale structures—with sufficient flux. The space available at BL-14A is not ideal, but it can be efficiently used for a SANS instrument (Figure 10). A sample area is foreseen to be slightly more restricted than the sample enclosure at EQ-SANS. The beamline could be placed in the space presently outside the building. The instrument hutch could be located on the second floor.

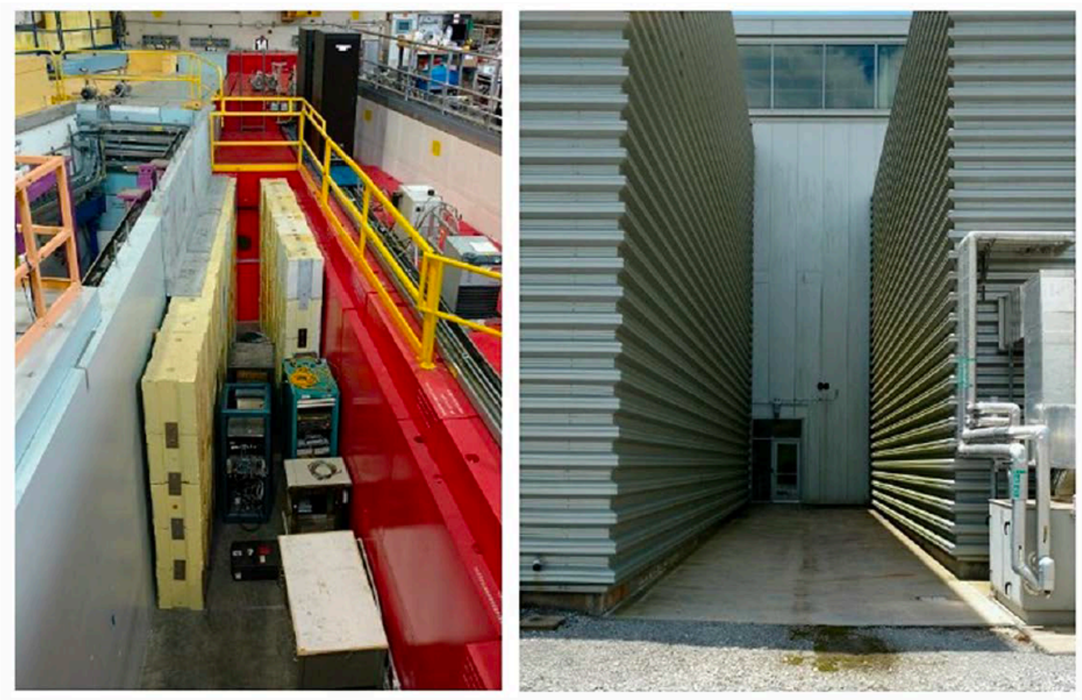

Figure 10. Space available at BL-14A for a possible SANS instrument. (left) Roughly 4 ft wide available space at the start of the yellow shielding blocks. Roughly 9.5 ft wide at the end of the BL-13 shield wall. (right) The outdoor space is ~14 ft along the entire length.

The space available at BL-14A is well suited to hosting a world-class 30–40 m GISANS instrument with a bandwidth of about 4 Å at 30 Hz operation mode. The extended length of the beamline would provide better Q resolution than EQ-SANS. The new beamline would also offer the opportunity to try new instrumentation concepts, including nontraditional detectors and detector arrangements and smaller guides optimized for smaller beam sizes.

Key Science Areas

Thin films and coatings play a vital role in our everyday lives, and their manufacture is now commonplace, while precise engineering of their performance remains challenging. Improved characterization methods have great potential for guiding these developments and improvements. GISANS instruments have great potential for contributing to our understanding of thin films because they enable probing structural features in films as a function of depth in the sample. At present, GISANS experiments are performed using available SANS and neutron reflectometry instruments; this strategy limits performance. Experiments presently require very long data acquisition times. Recent test experiments performed in EQ-SANS showed that, with appropriate beamline configurations, this time can be substantially reduced. Development of an optimized GISANS instrument would greatly benefit the community.

The benefits of GISANS would mainly manifest in soft condensed matter research, in which the contrast can be increased by way of sample deuteration. For inorganic applications, benefits of neutron over x-ray experiments may appear if magnetic contrast is present or if neutrons allow construction of more complicated sample chambers. A specific research area of interest is the static characterization and operando study of flexible electronics. An example for the latter is the study of interactions of particles with flow sensors in the body. This research requires sample environments that mimic the conditions in the body. Such experiments can be carried out with neutrons but are practically impossible for x-ray grazing incidence studies using x-rays in the 8–15 keV range, which is suitable for soft matter. An additional area of interest is the interface between polymer electrolyte and battery anode/cathode for the different types of lithium- and sodium-based batteries, especially because the electron density difference, and hence x-ray scattering contrast, between lithium and polymer is negligible.

An alternative proposed instrument for BL-14A, named INVENT, is designed to be an innovation platform for developing technology and methods that leverage improvements in source performance to maximize the science capabilities of the ORNL neutron sources. Its design could be similar to the NOBORU beam line at the Japan Proton Accelerator Research Complex. The flexibility and open sample access could support experimental campaigns that require combinations of extensive preparation time, complex (i.e., bulky) sample environments, or long measurement times as, for example, samples evolve in situ. This instrument could provide a flexible platform for assessing complex scientific apparatus (including pump-probe techniques and high magnetic fields) and for developing innovative technologies and techniques that are required for the transformative instrumentation envisioned for STS, FTS, and HFIR. While significant development activities proceed using modest development stations at HFIR, a strong and recurring need exists for an instrument station that provides pulsed neutrons with time-of-flight characteristics (i.e., moderator pulse shapes and spectral distribution) representative of FTS and STS beamlines.

Potential Instrument Relocations

Figure 7 shows three decision points that could potentially lead to relocation of instruments, thereby opening beam ports for future capabilities. These decisions involve the USANS instrument at BL-1A, the possibility of moving the SNAP instrument to make room for HighResPD, and the SNS-NSE instrument at BL-15. This section describes these three possibilities in detail together with the effects of these potential relocations.

Optimal location for USANS

The most likely future instrument relocation between facilities is the USANS instrument currently on BL-1A. USANS uses perfect single crystals of silicon and a Bonse–Hart technique that is frequently utilized in ultrasmall-angle x-ray scattering measurements. The optimization of such an approach for neutron scattering was pioneered at HFIR in the 1990s.[2] The instrument this team built at HFIR was previously installed on HB-3A thermal beam. During the last beryllium reflector change, the decision was made to utilize the HB-3A beam for a single-crystal diffractometer, which is now DEMAND. Plans to install a USANS instrument at HFIR following the cold source installation never materialized. Instead, a USANS instrument was installed at SNS at BL-1A. With years of operating USANS at BL-1A, the instrument performance is well understood, and a USANS instrument with much better performance can be built at HFIR.

As such, a team with representation from both NSD and NTD has been established to define a science case for a relocated USANS instrument, including benefits of co-location with the GP-SANS and Bio-SANS instruments and to estimate performance of the relocated instrument. The optimal beam location at HFIR has been identified as NB-2 (Figure 11), and we have discussed potential changes to the HBRR plans to accommodate this transition.

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[2] M. Agamalian, G. D. Wignall, and R. Triollo, "Optimization of a Bonse-Hart Ultra-Small-Angle Neutron Scattering Facility by Elimination of the Rocking-Curve Wings", *J. Appl. Cryst.* 30, 345 (1997).

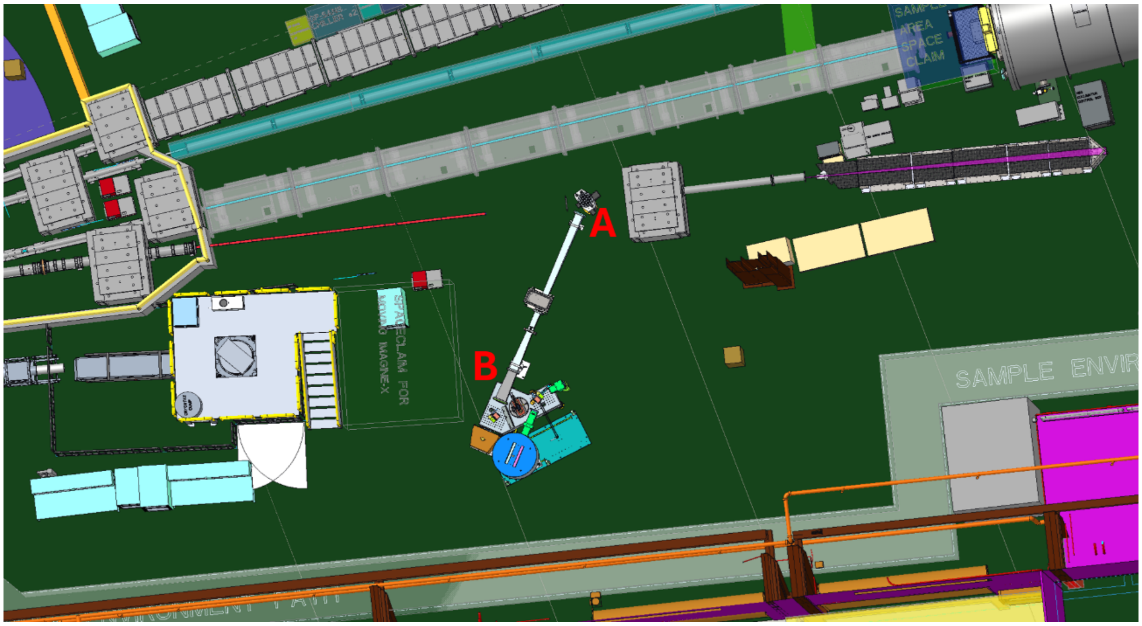

Figure 11. Potential location of the USANS instrument on NB-2 at HFIR following HBRR. The A location is the pre-monochromator location, and B is the nominal sample position. The distance between A and B can be shortened with minimal impact on performance. Therefore, adequate space is available at HFIR to accommodate the USANS instrument.

If the team concludes that significant gains can be achieved by moving USANS to HFIR, plans need to be developed to effectively utilize BL-1A. This beamline is shared with NOMAD, and space constraints impose restrictions on what can be located at this beamline. Possible instruments on BL-1A are in preliminary stages of discussion and may include the following.

SESANS

Spin echo small-angle neutron scattering (SESANS) is a technique that significantly surpasses the resolution of conventional SANS by extending the range of measurable momentum transfers. Unlike SANS, which directly measures momentum transfer via scattering angles, SESANS encodes momentum transfer into Larmor phase using precisely controlled magnetic fields. This method performs a Hankel transformation of $I(Q)$ to assess correlation functions in real space, rather than in reciprocal space as with SANS. SESANS can probe length scales beyond those achievable with traditional SANS, reaching scales comparable to those studied with Bonse–Hart USANS. This capability allows SESANS to conduct detailed investigations of long-range structures and interparticle interactions in a variety of systems, including colloidal dispersions, foams, lamellar fragments, supramolecular conjugates, complex mixtures, composites, and phase-segregated systems. The technique has promising applications in fields such as photonics, drug delivery, gene therapy, catalysis, separation science, and the development of next-generation materials.

Sample Alignment/Instrument Development

The BL-1A location could be modified in a straightforward manner to support single-crystal alignment or instrument development using a monochromatic beam. Currently, for the USANS instrument, a copper (111) pre-monochromator is used to deflect the beam. This beam could be utilized for crystal alignment by installing an appropriate goniometer and an area detector in the BL-1A instrument area. This upgrade may require replacing the copper (111) monochromator after more careful consideration of this use case. Ideally, an alignment station at SNS would utilize a white beam of neutrons, which is not possible on BL-1A. The same diffractometer could also be utilized for specific instrument development activities such as testing/aligning crystals for monochromator/analyzer assemblies at either SNS or HFIR.

High-Resolution Powder Diffractometer

A high-resolution powder diffractometer (HighResPD) on FTS has been specified to complement NOMAD, POWGEN, and DISCOVER by extending the resolution and, consequently, the detail at which powder crystalline materials can be explored. It will provide a high-resolution capability to the US science community with a $\Delta d/d$ resolution of 0.035%, matching the world's highest-resolution neutron diffraction instruments at the Japan Proton Accelerator Complex and the ISIS Neutron and Muon Source (United Kingdom). As described above, the HighResPD concept was endorsed by the IAB in 2018 with full understanding that it may require moving an existing instrument.

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

- Ab initio structure determination from powder diffraction (SDPD): With improvements in instrumentation, algorithm development, and enhanced computing power, great strides have been made in ab initio structure solution from powder diffraction data. Indexing and determination of space group is the first step in SDPD for which high-resolution data is required. The sensitivity of neutrons to light elements can play a crucial role in the determination of the correct space group, and therefore the correct interpretation of structure–property relationships.
- Addressing complexity and subtlety in functional materials such as zeolitic solids, piezoelectrics, ionic conductors, and others that have very large unit cell volumes and/or subtle structural distortions: This structural complexity is often integral to the useful physical properties of these materials. High-resolution data are needed to resolve subtle splitting in peaks or reveal subtle features in diffraction line shapes and to resolve an adequate number of Bragg peaks at high Q, where overlap and loss of information are significant issues for large unit cells.
- Magnetic ordering phenomena and magnetic coupling to other physical properties: Magnetic structures can often be extremely complex, requiring high-resolution data to resolve and distinguish long period modulation.

To implement such a capability, we need a beamline on a decoupled para-H_2 moderator and the ability to make a very long (approximately 100 m) instrument. Of the beamlines available, only BL-1A is on a decoupled para-H_2 moderator. Unfortunately, building a long instrument would be very difficult at that location because of facility infrastructure.

The remaining beam ports that view a decoupled para-H_2 moderator are BL-1B (NOMAD), BL-2 (BASIS), BL-3 (SNAP), BL-10 (VENUS), BL-11A (POWGEN), BL-11B (MANDI), and BL-12 (TOPAZ). BL-10, BL-11, and BL-12 are not compatible with a long instrument because such an instrument would interfere with STS on this side of the first target building. BL-1B has the same technical issues as BL-1A, and the current NOMAD instrument is the most productive instrument at SNS. BL-2 could accommodate a long instrument given that the BASIS instrument already has an 84 m incident flight path. No other locations are possible for BASIS at SNS, so the only possibility for BL-2 would be to replace BASIS with HighResPD. However, BASIS is the most productive neutron backscattering spectrometer in the world and frequently has one of the highest oversubscription rates of any instrument at SNS.

That leaves the possibility of BL-3. which has sufficient space to accommodate a long instrument. BL-3 is currently occupied by SNAP which is a compact instrument which could potentially be relocated. However, the SNAP beamline currently supports a world-leading high-pressure neutron diffraction program. Focused R&D in recent years has led to significant pressure cell development, and SNAP has performed neutron diffraction experiments in pressures up to 1 Mbar, which is world leading. Clearly, this instrument and capability are important, so plans for relocation must maintain or possibly expand current SNAP capabilities. The two potential open ports for a relocated SNAP are BL-1A and BL-8A. The latter would involve a change in moderator.

A working group will be established to consider the feasibility relocating SNAP and assessing the other decoupled-H_2 beamlines to determine what would be required to accommodate HighResPD.

BL-15 After a Spin-Echo Instrument Is Installed at HFIR

Plans for HFIR, described in the next section of this document, call for installation of a new spin echo spectrometer. Completion of this instrument raises questions about the future of SNS-NSE (BL-15). NSE capability is a scarce commodity worldwide, and the current situation at NCNR significantly limits the availability of this technique. Depending on the national situation at the time of completion of the HFIR spin echo instrument, SNS-NSE at BL-15 may need to keep operating to provide needed capacity to the user community. A similar approach was taken at Institut Laue–Langevin (ILL) over the course of many years, when the IN11 spin echo was kept operational alongside the IN15 spin echo, and the former instrument remained in demand and maintained a robust user program notwithstanding the much longer Fourier times accessible by the latter instrument. However, if a decision is made to replace SNS-NSE (BL-15) eventually, then it is logical to expect a new instrument at BL-15 to leverage the existing mu-metal enclosure, ideal for polarized neutron applications, which would be difficult and expensive to replicate elsewhere. A few possibilities of replacement instruments, such as SESANS and polarized diffractometer at BL-15, are presented in Figure 7.

HFIR Instrument Suite

The plans for HFIR over the next 10 years are dominated by the HBRR activity and associated AIPs. These projects have been developed in consultation with the user community and guided by several focused reviews. These reviews have made specific recommendations for HFIR instrumentation that have fed into our plans and strategy. As with SNS, one important activity was the IAB which included the following recommendations:

- "The IAB recommends that ORNL update and optimize the thermal neutron instrument suite at HFIR to provide the US neutron community with internationally competitive instrumentation."
- As part of the upcoming beryllium reflector change, the IAB made the following recommendations:
    - "The IAB recommends that ORNL develop a national roadmap for NSE." Focus of this discussion was on developing a neutron spin echo at HFIR to enable measurements at Fourier times consistent with IN15 at ILL.
    - "The IAB believes that ORNL should develop a modern guide and the primary spectrometer for a new cold triple-axis spectrometer."
    - "The IAB believes that the new cold guide system should not degrade the performance of the cold imaging station and should enhance it if possible."

HFIR Cold Guide Hall

An optimization activity followed this review to determine whether it was possible to design a cold guide network at HFIR to enable a high-resolution NSE instrument, a world class cold triple-axis spectrometer, and preserving the capabilities of the cold neutron imaging station. This resulted in a transition from a four-guide network to a six-guide network providing two new end stations and an extension of the cold guide hall. The new instrument layout is shown in Figure 12.

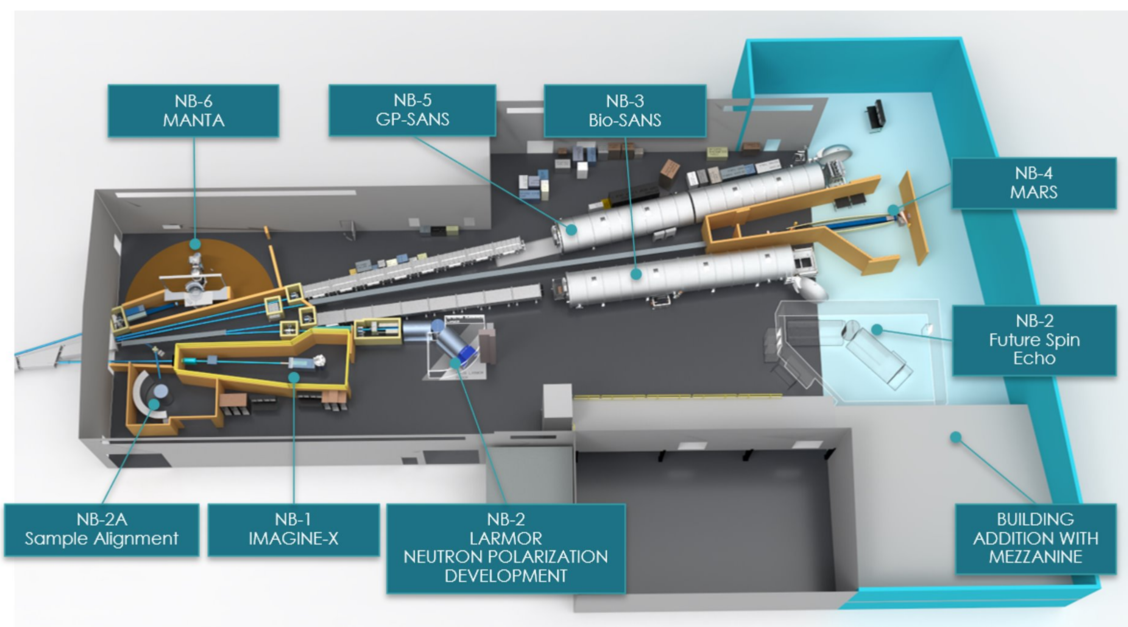

Figure 12. Expanded HFIR cold guide hall (light blue shows the expanded region) and instrument layout with six guides (NB-1 to NB-6).

Note that the guide number is changing handedness (e.g., the current CG-1 is close to the new NB-6 location and the current CG-4 is close to the new NB-1 location). With this terminology change, Table 5 summarizes the instrument reconfiguration in the guide hall:

Table 5. Summary of instrument reconfiguration in the HFIR cold guide hall.

Current instrument	New instrument	Notes
Crystal alignment (CG-1B)	Crystal alignment (NB-2A)	Double-bounce monochromator to bounce over the NB-1 guide
Detector Test Station (CG-1A)	Capability moved to POPLAR (HB-2D)	
MARS (CG-1D)	MARS (redesigned) (NB-4)	Instrument relocation enables moving the MARS cold neutron imaging instrument to a location between the two SANS instruments
GP-SANS (CG-2)	GP-SANS (NB-5)	GP-SANS is moved slightly downstream
Bio-SANS (CG-3)	Bio-SANS (NB-3)	Bio-SANS is moved slightly downstream and away from GP-SANS to make room for MARS
Polarized development (CG-4B)	Temporary PILOT instrument (NB-2C)	PILOT will be installed on NB-2 and utilized until funding is secured for the neutron spin echo instrument.
N/A	High resolution neutron spin echo (NB-2)	When funded, this instrument will replace the PILOT development beamline
CTAX (CG-4C)	MANTA (NB-6)	Modern cold triple-axis spectrometer with 50× the flux of CTAX and designed to enable implementation of a multianalyzer secondary spectrometer
IMAGINE (CG-4D)	IMAGINE-X (NB-1)	IMAGINE-X will incorporate dynamic nuclear polarization and Anger camera detectors. Move to NB-1 is expected to double the flux on sample
N/A	USANS (NB-2B)	USANS working group analyzing this possibility

Figure 13 provides another view of the instrument reconfiguration in the cold guide hall and modifications planned in the thermal beam room.

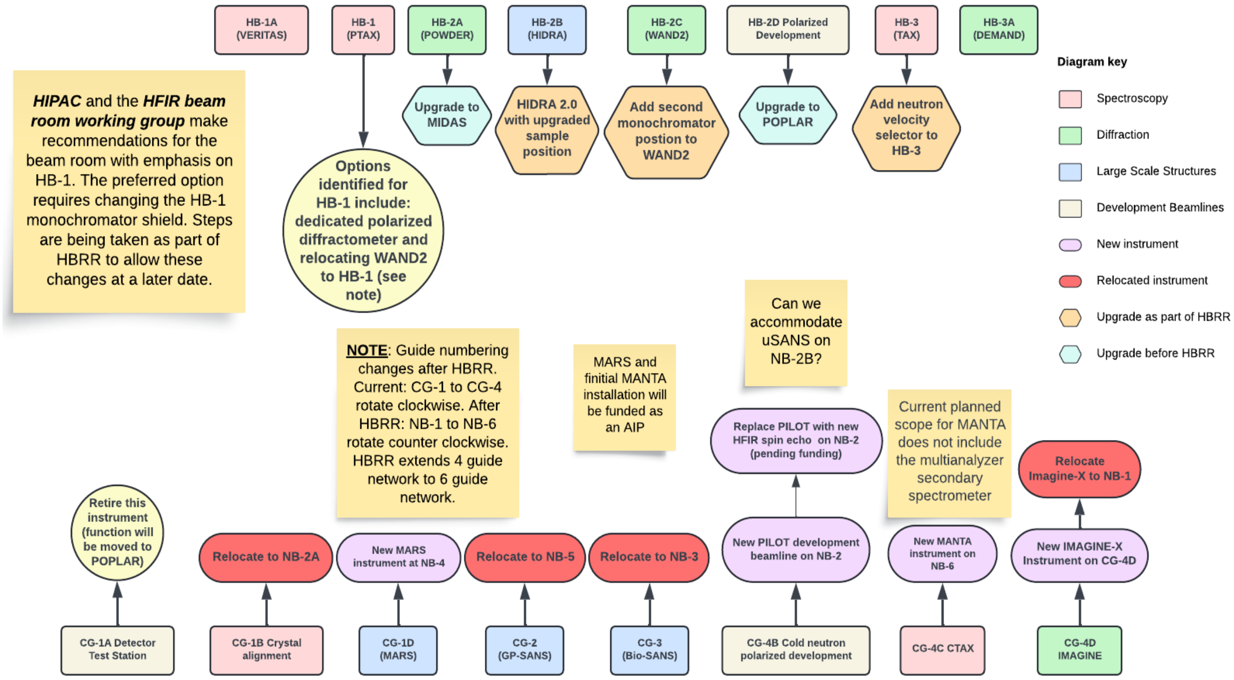

Figure 13. Diagram showing possibilities for future instruments at HFIR following HBRR and related AIPs

New or Significantly Modified Instruments

IMAGINE-X

A funded BRaVE proposal led by Dean Myles will result in IMAGINE being replaced by IMAGINE-X (project completion expected by August 2026). The IMAGINE neutron image plate diffractometer is designed for rapid collection of high-resolution (~1.1 Å) Laue or quasi-Laue data from small single crystals (>0.1 mm^3) of moderate unit cell size (~100 Å), primarily for structural biology. The IMAGINE-X project has two major instrumentation components:

1. Integrating dynamic nuclear polarization (DNP).
2. Replacing the current image plate detectors with an array of 2D position-sensitive Anger cameras based on silicon photomultiplier tube technologies, which makes then magnetic field insensitive.

The net result of this upgrade will be an enhancement of the instrument's sensitivity to hydrogen atom positions (without the need for deuteration) and a significant reduction in crystal size requirements. The project will also develop new software for data indexing, data collection, data processing and analysis of DNP-enhanced diffraction data, and an integrated digital twin platform to steer and control the experiment. Relocation of IMAGINE-X to NB-1 (Figure 14) will increase flux (expected gain of a factor or 2), reduce beam divergence, and optimize the neutron wavelength cutoff. Ultimately, this upgrade will enable studies of many more proteins and other biomacromolecules that are not feasible today.

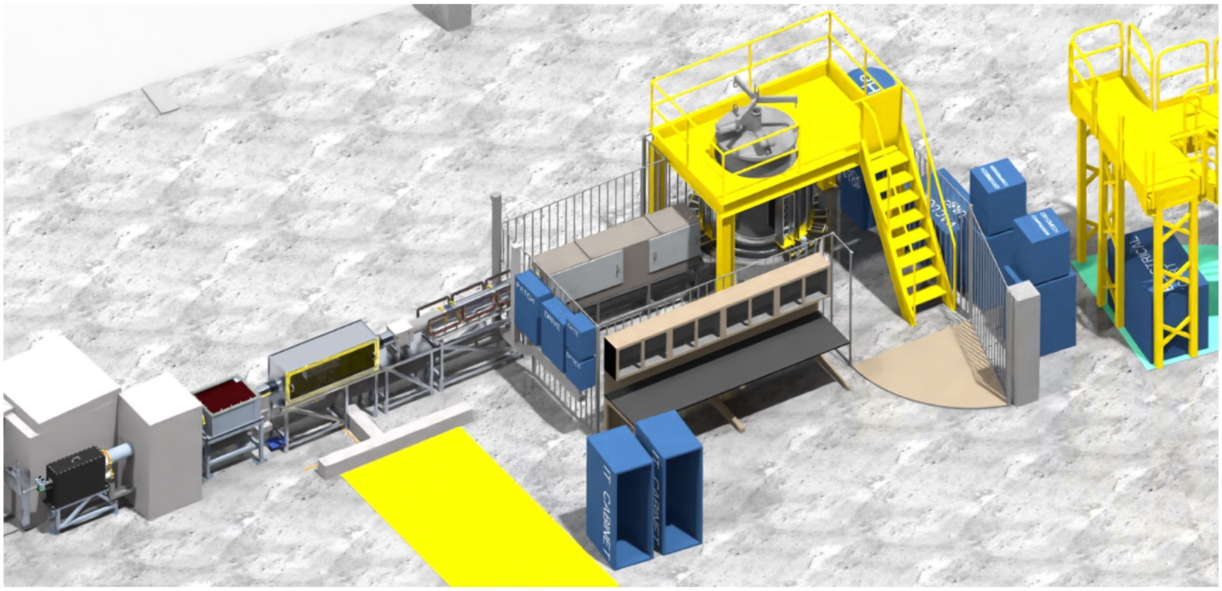

Figure 14. Engineering drawing of the IMAGINE-X beamline after HBRR.

In addition to the ongoing IMAGINE-X project, the new HFIR cold guide network will enable the following three new instruments, which are consistent with the guidance of the IAB.

MANTA

MANTA will be a world-class cold neutron triple-axis spectrometer located at HFIR. Following the HBRR activity, the CTAX (CG-4C) instrument will be replaced by MANTA, which will move to the new NB-6 beamline. The incident beamline of this new spectrometer has been optimized[3] and will incorporate a multichannel guide with horizontal focusing, a neutron velocity selector, the ability to accommodate an incident beam polarization, and a double-focusing PG (002) monochromator. The resulting optimized optics result in a flux of ~10^8 n/cm^2/s on a sample with an area of 2 cm × 2 cm (Figure 15).

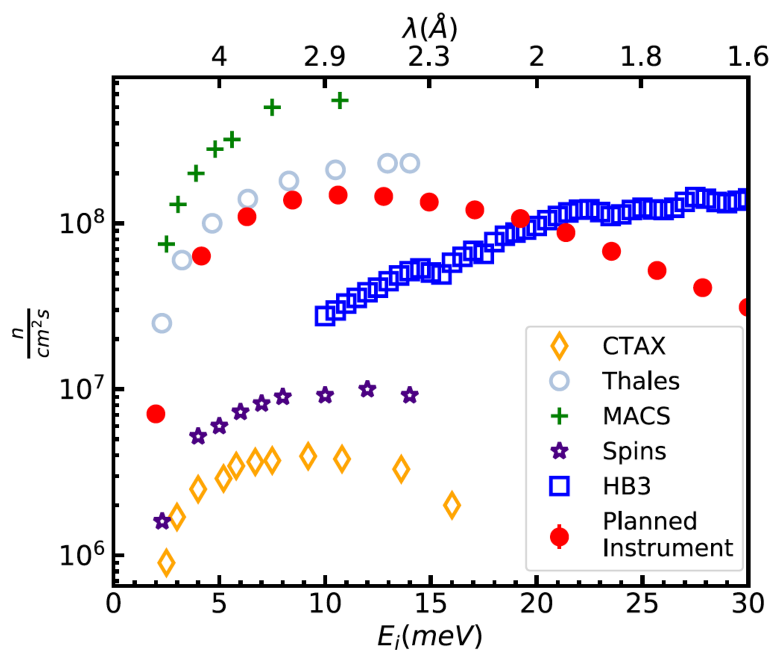

Figure 15. Neutron flux on sample for MANTA compared to other cold triple-axis spectrometers.[3]

The secondary spectrometer of this instrument will be exchangeable and will include a conventional single analyzer/detector configuration repurposed from CTAX and a massively multiplexed secondary spectrometer for survey measurements.

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[3] G.E. Granroth et al., NIM-A 1064 169440 (2024) dx.doi.org:// j.nima.2024.169440)

The multiplexed spectrometer has not been fully designed at this point but will likely be similar to the design currently employed at the CAMEA instrument at the Paul Scherrer Institut or the recently proposed MARMOT concept (silicon (111)-based CAMEA concept). The incident beam optics, monochromator drum, new monochromator, floor, and repurposing of the current CTAX secondary spectrometer will be funded as an AIP. The full multianalyzer secondary spectrometer will require additional future funding. Following discussions with colleagues in Japan and an experiment by ORNL staff at JRR-3 using the HODACA instrument, it has been decided that a similar concept could be utilized as an interim multianalyzer configuration. This gives good coverage at a single final energy but doesn't provide multiple final energies. This secondary spectrometer is much more compact and can utilize single tube detectors available after completion of the MIDAS project on HB-2A.

The MANTA instrument concept and science case have been developed with input from the user community. Two MANTA-focused workshops were held at ORNL in 2015 and 2017 to establish scientific needs and discuss instrument parameters. MANTA was presented at both triple-axis suite assessments and was identified as the highest priority. As mentioned previously, MANTA was recommended by the IAB. Aspects of MANTA were presented to the user community at ACNS meetings in 2018, 2020, and 2022. Our Japanese collaborators have been engaged in the MANTA project through the annual meetings of the US-Japan Collaborative Program on Neutron Scattering.

Neutron Spin Echo

The NB-2 guide profile, and intensity makes it most suitable for a spin echo spectrometer that focuses on low-*Q* measurements suitable for the soft-matter and biophysical user communities. The spectrometer will provide access to longer Fourier times via the use of longer wavelengths available from the cold source at HFIR, and new superconducting technologies and improved magnet designs will be used to deliver the optimum beam at the sample. The HFIR-NSE spectrometer could reach Fourier times of 100 ns at a wavelength of $\lambda = 8$ Å with a neutron flux that will greatly reduce the measurement times of a typical experiment. The availability of longer wavelength at HFIR, $\lambda > 8$ Å, will further expand the accessible range of Fourier times because they scale as λ^3. Typical HFIR-NSE applications will include thermal fluctuations and relaxation phenomena in polymer networks and polymer melts, interface fluctuations in complex fluids and polyelectrolytes, transport processes in polymer electrolytes and gel systems, domain fluctuations in proteins and enzymes, lipid systems and biological membranes, disruptive effects of medication on membrane cell organization, and transport processes through cell membranes and porous media. A new NSE spectrometer with these capabilities can be achieved with conventional DC or RF fields, and ORNL is currently conducting a strengths, weaknesses, opportunities, and threats analysis of these two technologies to establish a path forward.

MARS

Given the new, dedicated NB-4 guide, the Multimodal Advanced Radiography Station (MARS) will be a purpose-built high-flux, cold neutron imaging instrument hosting a wide range of imaging modalities, including radiography, tomography, polarized imaging, and grating interferometry. Compared with the existing configuration, the flux on sample will be enhanced by at least a factor of 10, the beam profile will be more uniform as necessary for high-resolution imaging, and the now completely shielded cave will be more spacious to accommodate complex sample environments. Furthermore, a new upstream velocity selector and rebuilt double-bounce monochromator will allow for selective neutron wavelengths for enhanced image contrast and will enable quantitative neutron grating interferometry measurements. Future upgrades will include a compact x-ray source for simultaneous neutron and x-ray imaging (*SNAX)*, dedicated polarization setup, and advanced neutron optics such as Wolter mirrors. These capabilities complement the time-of-flight instruments VENUS (SNS FTS) and future CUPI^{2}D (SNS STS).

HFIR Thermal Beam Room

The HIPAC reviewed plans related to HBRR. They strongly endorsed the new six-guide network in the guide hall. Like the IAB, this committee made recommendations about focusing on modernizing and optimizing the thermal neutron instrument suite at HFIR. To follow up on this report, the internal HFIR Beam Room Optimization Working Group was formed to discuss the thermal neutron instruments at HFIR with particular emphasis on the thermal triple-axis spectrometers. This working group identified specific options to optimize beam room instruments:

1. Maintain the HB-1 and HB-3 triple-axis spectrometers but upgrade the monochromator drums to improve the overall instrument layout and enable future developments.
2. Merge the polarized and unpolarized thermal triple-axis capabilities on HB-3. The following two options were identified for HB-1:
    a. Move the WAND^2 instrument to HB-1, allowing for variable incident energy.
    b. Develop a new fully polarized diffractometer on HB-1.

The committee had strong preference for option 2b above to enable continued development of advanced polarization techniques, such as the Wollaston prisms, providing Larmor diffraction capabilities and spherical neutron polarimetry to elucidate complex magnetic structures. These two developments were supported by DOE Early Career Awards and require a fully polarized diffractometer to deploy them to the user community. To enable the preferred option, the monochromator shield on HB-1 would need to be replaced. One identified option for this task would be a double-bounce monochromator assembly, which enables variable incident energy and provides the ability to better optimize space in the beam room (which is particularly important for a versatile instrument with multiple polarized neutron capabilities).

The HBRR planning and current budget does not allow this preferred option to be implemented. However, we have carefully considered the HBRR plans to ensure that such an upgrade would be possible in the future. As such, HBRR will only enable modest upgrades to the thermal neutron instrument suite, and these upgrades are described in the following subsections.

HBRR Opportunistic Upgrades

HIDRA 2.0

The HIDRA 2.0 upgrade (Figure 16) details the addition of a six-axis robot arm for manipulation in *XYZ* as well as ΨΦ, which are required for determination of a full second-rank strain tensor. Neutron diffraction studies of materials under applied stress reveal phase-level and grain-level knowledge of deformation processes, which are fundamental for developing finite element and self-consistent field models of materials behavior. Additional systems of relevance for this instrument include functional materials in varied environments, such as piezoelectric materials in applied fields and shape-memory alloys under varying load and temperature conditions.

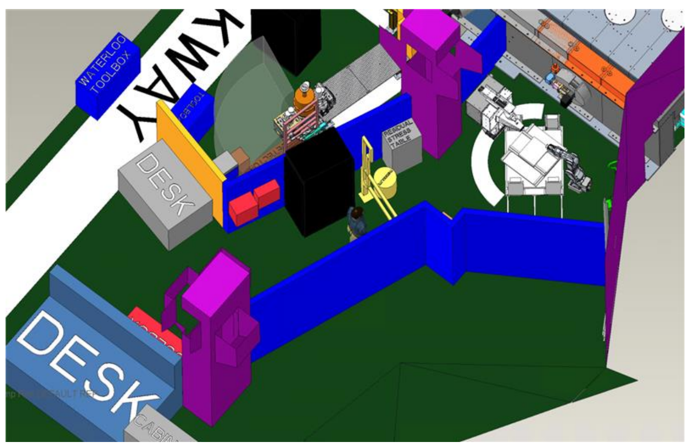

Figure 16. HIDRA instrument at the completion of HBRR.

The upgrade involves the following:

1. Additional shielding for background reduction

2. Three-axis (*XYZ*) goniometer with integrated high weight-capacity *Z* motion
3. Six-axis robot arm for small (<15 kg) sample manipulation

These upgrades are crucial for HIDRA to remain world class in the next decade and meet the demands of the user community to better characterize advanced materials and advanced manufacturing processes. The shielding is required because of the beam room's high background, which can change during an experiment at HB-2B. Figure 17 shows the change in the background seen on the HB-2B detector based on the configuration of the HB-3 instrument. This instrument crosstalk can be seen in our data. Proper shielding should be explored to reduce this effect and allow smaller gauge volumes at HIDRA (<1 mm). The upgraded *XYZ* goniometer with integrated high-capacity (~700 lb) *Z*-stage is needed for sample environments at HB-2B such as the creep electrostatic levitator, the HFIR load frame, and spatial mapping in furnaces/cryostats. A six-axis robot will allow for texture mapping and full tensor mapping required for characterization of materials made via additive manufacturing where the principal strains are not known a priori.

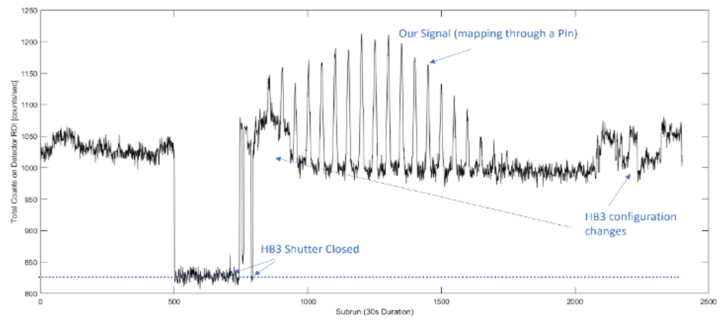

Figure 17. Background changes over time at HB-2B. Total counts on detector are plotted versus each 30 s measurement. Both when the HB-3 shutter is closed as well as when the instrument changes collimation and configuration can be seen in the intensity.

Second WAND[2] Monochromator Position

During HBRR, the HB-2 shielding tunnel will be redesigned and rebuilt, providing a unique opportunity to consider adding capabilities. Currently, WAND[2] has a fixed monochromator scattering angle of 50°. The post-HBRR WAND[2] instrument will include a second monochromator position at a much higher scattering angle. This upgrade will allow the instrument to switch between a higher flux, lower resolution configuration and a lower flux, higher resolution configuration, resulting in a highly flexible and versatile instrument.

Neutron Velocity Selector on HB-3

The monochromatic neutron beam selected by Bragg reflection contain higher harmonics (i.e., λ/n) for certain monochromator choices including the preferred PG (002) crystal. These higher harmonics are a source of considerable background for both HB-3 and neighboring instruments such as HIDRA and DEMAND. To eliminate these neutrons and reduce instrumental background, a project was proposed and prioritized in FY 2016 to procure and install a neutron velocity selector before the monochromator. The velocity selector was purchased and received at ORNL. However, full installation involves rebuilding the cubicle, designing a new instrument shutter, and moving the drum slightly away from the reactor shielding face. The complexity of this installation makes it advantageous to couple this activity with HBRR. This upgrade must also be coordinated with the proposed DEMAND Beamline Extension project because the HB-3 cubicle modifications must be compatible with the HB-3A (DEMAND) plans.

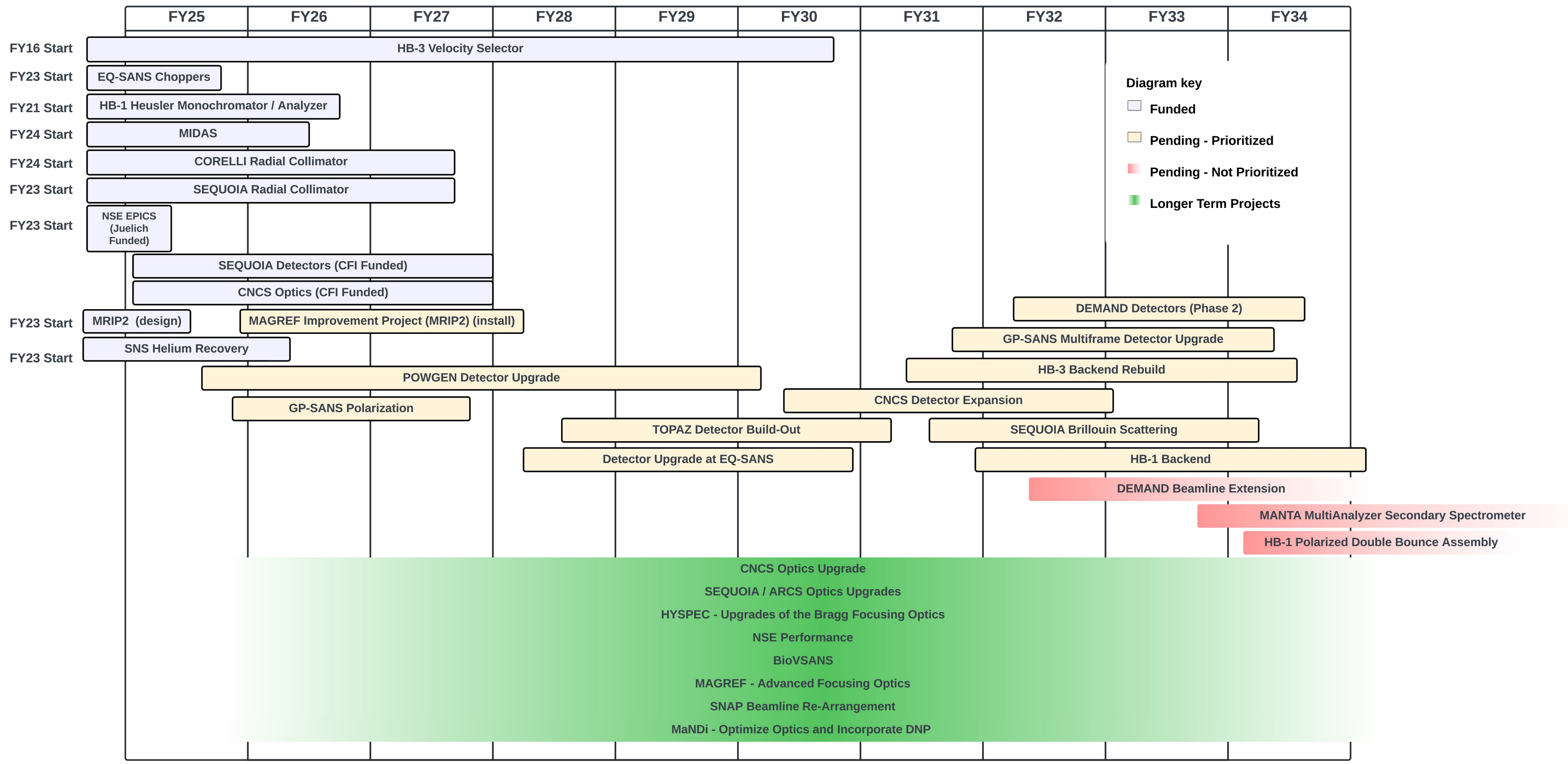

Figure 18. Notional timeline for instrument upgrades, including funded projects, projects that have been prioritized but not currently funded, and projects that are not currently prioritized. Longer term projects are listed (in green), but these often require significant R&D. As such, they may not even develop into full projects or may become highly prioritized, depending on the outcome of these R&D activities. Consequently, they are listed across the entire time period of this timeline.

Upgrades

The directorate invests operational funds to keep the current instruments competitive and optimized via upgrade projects. The process for reviewing and prioritizing these upgrades is described in the Prioritization Processes section of this document. The following section describes some of the recent upgrades that have been delivered by this process, upgrades that are currently underway, those that are prioritized but not yet funded, and projects that are not recommended at this time. The same process is used to prioritize large sample environment investments, but these are not included in this document. Additionally, this section ends with a description of some longer-term upgrades under consideration across the instrument suite. The upgrades described below are included on a notional timeline in Figure 18.

Recently Completed Upgrades

NOMAD Detectors

Cost: $2.76 million

The NOMAD instrument detector arrangement consists of six sections; a forward scattering bank, a backscattering bank, and four banks arranged in a cylindrical geometry around the sample position (referred to as the ring detector banks). Before this upgrade, all banks were about 50% populated. This upgrade completed all four ring detector banks with new 1 in. ^{3}He tubes, and the electronics on all detectors were updated to current technology. In addition to the new detectors, 3D printed coarse collimators were installed in front of all the ring detectors to reduce secondary scattering from sample environments. Overall, the upgrade nearly doubles instrument throughput, enables texture and preferred orientation measurements, and enables measurements for single-shot time-resolved studies, transient structures, and samples with limited lifetime.

VULCAN-X

Cost: $4.36 million

VULCAN-X Phase 1 resulted in replacement of the original VULCAN detector technology on the primary 90° detectors with new ^{3}He tube arrays and provided 2× higher counting rate, 10× finer spatial resolution in the vertical direction, and greatly reduced sensitivity to gamma background. VULCAN-X Phase 2 added additional detector banks for greater angular coverage. The instrument now has a total of six banks (768 ^{3}He tubes), and detector angular coverage is more than doubled. The highest data rate exceeds 20 million counts per second. The investments ensure VULCAN's continued leadership in rapid measurements of material response and behavior under extreme and complex operando environments, such as a running engine or additive metal manufacturing processes. The upgrade also enables new science applications under extremes, such as grain orientation-dependent evolution in lattice strain, damage, and phase transformation.

SNAP Optics

Cost: $1.31 million

New focusing mirror guides and motorized beam optics table delivers a threefold improvement in flux, reduced background, reduced divergence, and improved peak shapes, as well as improved performance, reliability, and flexibility to reconfigure for imaging applications. This upgrade enables smaller samples, improved Rietveld analysis, new diamond anvil cell and single-crystal experiments and the development of the time-of-flight imaging program (which will move to VENUS upon completion).

HYSPEC Analyzer Elevator

Cost: $0.22 million

An elevator was added to HYSPEC to enable automated changes between the polarizing supermirror analyzer and the radial collimator. This upgrade also adds an oscillation capability and the ability to adjust the orientation of the polarizing supermirror. This capability enables easy transitions between unpolarized and polarized operations which is frequently requested by users and the ability to optimize transmission through the polarizing supermirror array.

VERITAS

Cost: $3.18 million

(update: 12/16/24: scope complete – additional funds approved for integration of a single Anger camera)

This upgrade improved the incident optics and replaced the secondary spectrometer. Replacing the incident monochromator and PG filter resulted in a 3× increase in flux on sample. The secondary spectrometer rebuild was optimized for reduced background and improved divergence acceptance. Overall, this upgrade resulted in significant improvements in signal-to-noise (factors of 5–10) and enabled the addition of new capabilities, including a four-circle goniometer and a 2D Anger camera position sensitive detector, expanding the science that can be performed on the instrument.

SANS Collimator Upgrade

Cost: $3.8 million

The movable collimator sections of the two HFIR SANS instruments (GP-SANS [CG-2] and Bio-SANS [CG-3]) were replaced. The replacement included new vacuum housing, support structure, shielding and guide/aperture positioning stages. At the same time, these beamlines were converted to a new Experimental Physics and Industrial Control System (EPICS)-based instrument control system. The upgrade increased operational reliability by replacing mechanical feedthroughs with in-vacuum motors. It also improved data quality with reduced low-angle background around the direct beam. Furthermore, the new collimator boxes provide greater flexibility for adding future optional optical elements, such as focusing lenses.

Bio-SANS Detector Upgrade

Cost: $0.96 million DOE Biological and Environmental Research (BER) Funded

(update: 12/16/24: all scope complete)

This upgrade expanded the Bio-SANS detector coverage by adding two ^{3}He tube area-detector arrays (west wing and mid-range) to the central main detector, more than doubling the active detector area. It enables simultaneous coverage of a wide angular range (dynamic Q range [i.e., $Q_{max}/Q_{min} \approx 300$), and greatly improves capabilities for time-dependent in situ studies of hierarchical systems over a wide range of length scales. The beamline pioneered this approach at reactor-based SANS instruments and was first to provide such a wide range of angular resolution in a single shot.

Ongoing Funded Projects

HB-1 Heusler Monochromator/Analyzer

Cost to date $0.42 million, Total estimate: $1.005 million

The previously purchased Heusler crystals are not of good quality and limit the instrument performance. This upgrade will replace the Heusler monochromator and analyzer crystals with previously used crystals from the now closed facility at the Laboratoire Léon Brillouin in France. This upgrade will significantly improve neutron polarization and flux, enabling experiments that currently cannot be performed in the United States.

MIDAS

Cost: $2.9 million

(update: 12/16/24: install likely delayed by ~6 months to end-of-cycle 518 (4/24/26) due to lead time on collimator, DAQ availabilities, and craft resources)

The MIDAS project will replace outdated and inefficient point detectors with position-sensitive detectors. This upgrade will decrease measurement times by a factor of nearly 30 by removing the need to step through gaps between detectors. Improved counting times enable the extended use of pressure cells, polarization measurements, diffuse scattering studies, and improved throughput. Additionally, this upgrade will expand the instrument into new science areas, including in situ studies.

EQ-SANS Choppers

Cost: $1.08 million

Installing two double disc choppers will provide more flexible wavelength selection and wavelength resolution for time-of-flight SANS, reducing inelastically scattered neutron effects and improving the quality and fidelity of the data provided by EQ-SANS.

CORELLI Radial Collimator

Cost: $0.50 million

(update: 12/16/24: small additional increase needed to address safety concerns when VIT is removed)

A fine radial collimator is needed for CORELLI to support general sample environments including high-field superconducting magnets, orange cryostats, ultralow-temperature inserts, and closed-cycle refrigerators. This upgrade will enable the study of magnetic phase transitions and spin structure determination under high magnetic fields. The lower background will also enable measurements that are currently challenging on small-sized single crystals (~1 mm^3)

SEQUOIA Radial Collimator

Cost: $0.74 million

This project will design, fabricate, and install a radial collimator between the sample and detectors on SEQUOIA. This upgrade will significantly reduce background without reducing signal, thereby greatly improving signal to noise with large sample environments, such as high-field magnets.

NSE EPICS Upgrade

Cost: $0.67 million; Funded by SPP with Jülich

NSD took over the SNS-NSE beamline after the completion of the instrument development team agreement between ORNL and Forschungszentrum Jülich, Germany. Jülich provided project close-out funds of $700,000 for acquisition of hardware, which helped convert the beamline from obsolete and Jülich-specific instrument components and control hardware to systems that are standard at SNS. The upgrade ensures that NSD maintains this unique capability of the finest energy resolution spectroscopy technique.

SEQUOIA Detectors

Cost: $2.3 million; Funded by Canada Foundation for Innovation

The SEQUOIA detector tank was built to support five rows of ^{3}He position-sensitive detectors, but only three rows are currently populated. Expanding the full detector array will significantly increase the detector coverage, resulting in performance gains for most experiments. This project will be funded by a Canada Foundation for Innovation grant with Bruce Gaulin, McMaster University, as the principal investigator.

CNCS Optics

Cost: $0.48 million; Funded by Canada Foundation for Innovation

This project will add new neutron optics between the high-speed double disk chopper and the sample position and enable automated changes between components. This upgrade will eliminate a bottleneck in adapting optics to the experiment. The team is considering a short vertical focusing device based on nested mirror optics to improve flux on sample for large sample environments such as the 14 T magnet (in consultation with SwissNeutronics). Overall, this project will improve efficiency and performance for specific experiments. This project will be funded by a Canada Foundation for Innovation grant with Bruce Gaulin, McMaster University, as the principal investigator.

MAGREF Improvement Project Phase 2 (MRIP2)

Cost: $2.36 million

This project upgrades the pre-sample optics bench to improve efficiency and reliability, improve data quality, optimize polarization handling, and add a new capability to perform polarized reflectivity imaging. This project will enable the future use of higher-M polarizers and higher applied magnetic fields at the sample. Only initial design activities are currently funded. Full completion of the project is not yet funded.

SNS Helium Recovery

Cost: $1.77 million

Liquid helium (LHe) cost and availability negatively affects our operating budget (the cost of LHe) and the feasibility of low-temperature and magnetic field experiments. This proposal will begin to address both local and facility-wide collection, purification, and liquefaction of LHe. The annual consumption of LHe is approximately 22,000 L/year at HFIR and 17,000 L/year at SNS. The cost of LHe is currently $34/L, and this price has doubled since 2021. This project will provide a facility solution for SNS that can and will be expanded for use at all beamlines at both facilities as well as other LHe users at ORNL. This solution collects and compresses helium off-gas into a central tube trailer. The helium is then transported to the SNS LINAC test station for purification, liquefaction, and filling of LHe dewars.

Prioritized but Not Funded

This section includes a list of projects that have been prioritized by the SPSC but are awaiting funding. The listed costs for these projects are approximate.

POWGEN Detector Upgrade

Cost estimate: $4 million

This upgrade will complete the POWGEN detector coverage with GEN-II detectors. The newly developed GEN-II detectors will improve instrument resolution by about 25% and will increase total counting rate by about 2.8×. The additional coverage, count rate, and resolution will enable new science capabilities (e.g., complicated/weak magnetic structures, extremely small samples, and microstructure analysis). Further work in hardware and software could further increase resolution.

GP-SANS Polarization

Cost estimate: $0.42 million

This project involves installing and aligning a polarizer and magnetic yoke in upstream collimator Box 1, installing guide fields along length of the collimators, and installing a breadboard mount for a spin flipper in the sample area. The upgrade will provide a new capability, making polarized SANS available to the HFIR/SNS neutron user community. It will allow users at GP-SANS to use half-polarization whenever needed in their experiments because the capability will be installed and an available option all the time. User communities that will benefit from the investment are primarily in quantum materials, but biology, soft matter, and engineering materials could also benefit from having access to polarization at GP-SANS.

GP-SANS Multiframe Detector Upgrade

Cost estimate: $4.2 million

With the current scarcity of neutrons in North America, there is a large user-driven need for more SANS beam time. To ease the burden of oversubscription, we need to make experiments more efficient so that beam time is used as effectively as possible. The proposed upgrade enables that capability for the kinetic studies that GP-SANS is doing more often in a multitude of science areas and fosters a better mail-in program. This project can take advantage of the proposed cold source downtime before the longer HBRR shutdown. Installing and commissioning the detectors before the instruments are down for a year or longer will yield two major benefits. (1) GP-SANS can hit the ground running after HBRR with minimal commissioning time, and (2) the instrument and software teams will have a year to work on user interfaces to the new multiarray detector. The diffraction community that uses GP-SANS predominantly use the GrASP software package, but after this upgrade, it will not be an option. The teams will need time to develop new visualization tools and workflows to interact with these data, especially in multiple dimensions.

HB-3 Triple-Axis Backend Rebuild

Cost estimate: $2.4 million

The current HB-3 backend has limited vertical and horizontal acceptance, low data collection efficiency, and inadequate shielding, and it imposes limitations on the weight carried by the sample table. A redesigned HB-3 backend will increase the signal-to-noise ratio and allow the use of larger and heavier sample environments, including higher magnetic fields. The new design will provide a greater horizontal and vertical acceptance of the scattered beam and will allow the use of horizontal focusing. This upgrade will enable experiments that are not feasible today owing to the high instrumental background, which limits signal to noise.

DEMAND Detectors (Phase 2)

Cost estimate: $1.2 million

This upgrade will complete the three-column detector build-out by adding two additional columns, tripling the DEMAND detector coverage and accelerating data collection by 2–3 times. It will serve to support a larger user community by efficiently measuring larger unit cell compounds, such as metal–organic frameworks and molecular magnets.

CNCS Detector Expansion

Cost estimate: $1.88 million

This upgrade will complete detector configuration at CNCS using detectors from an instrument that was decommissioned at the Lujan Center at Los Alamos National Laboratory, doubling the instrument detector coverage for improved measurement efficiency for out-of-plane scattering.

SEQUOIA Brillouin Scattering

Cost estimate: $0.7 million

The addition of a low scattering angle detector (<2.5 deg), an incident beam chopper, and collimator system will result in a new Brillouin scattering capability for crystalline or amorphous materials and liquids. One use case for this capability is the study of new, rare earth–free ferromagnets. With the Brillouin scattering option, the spin wave spectrum can be measured effectively in polycrystalline samples.

TOPAZ Detector Build-Out

Cost estimate: $2 million

Detector buildout for 21 unoccupied ports using the field-insensitive silicon-based Anger cameras will complete the detector array on TOPAZ. This upgrade will enable experiments in the presence of high magnetic fields and polarized neutron diffraction measurements, will increase the data collection efficiency, and improve the spatial resolution.

HB-1 Backend Upgrade

Cost estimate: $1.65 million

This project is designed to build a new secondary spectrometer to deliver high beam intensity, good polarization, and increased flexibility. It incorporates larger beam windows to increase intensity, nonmagnetic materials for optimal polarization, and extendable arms before and after sample table for higher resolution. It will deliver higher quality data and enhanced performance for state-of-the-art devices, such as Wollaston prisms, and spherical neutron polarimetry.

Detector Upgrade at EQ-SANS for Extended Dynamic Range

Cost estimate: $4.2 million

This proposal aims to enhance the detector system of EQ-SANS through two main upgrades. Firstly, the current primary detector, consisting of 1 m long ^{3}He linear position-sensitive detectors arranged in staggered planes, will be replaced with a single flat array. This modification will simplify corrections required for data reduction. Secondly, medium- and wide-angle banks of detectors will be added to the instrument to provide more complete wavevector coverage, aligning it with modern SANS instrument designs. We expect wide Q ranges from 0.006 Å^{-1} < Q < 1.2 Å^{-1} to 0.002 Å^{-1} < Q < 0.3 Å^{-1} can be accessible, depending on the choice of wavelength bands (minimum wavelength of 2.5 Å and 10 Å, respectively). These upgrades will not only improve instrument throughput but also expand its capability for performing cutting-edge time-resolved SANS experiments.

Other Projects Considered by the SPSC but Not Currently Prioritized

The following projects have been considered by the SPSC but are awaiting the HBRR plan to be finalized before final prioritization is determined. Budget information is not included because of the early phase of these projects.

MANTA Multianalyzer Secondary Spectrometer

An AIP will be funded to install the incident optics on NB-6, resulting in world-class flux on sample for a cold triple-axis spectrometer and a 50× improvement over the current CTAX instrument. An additional project is required to realize the ultimate plan for this spectrometer. This project will involve design and fabrication of a state-of-the-art multianalyzer secondary spectrometer, which will be informed by other international efforts to design such secondary spectrometers, including the currently installed CAMEA instrument at the Paul Scherrer Institut, HODACA at the Japan Research Reactor-3, and the proposed MARMOT concept at ILL. Additional capabilities and capacity for cold neutron spectroscopy are a frequent request from the quantum materials user community, and this multianalyzer secondary spectrometer will greatly improve efficiency.

DEMAND Beamline Extension

DEMAND is a key diffractometer to investigate novel magnets and materials. It is also a unique magnetic polarized single-crystal neutron diffractometer at ORNL to study magnetic anisotropy, spin-orbital coupling, and magnetic interactions that are critical for investigation and design of new quantum and molecular magnets. This project will move the beamline farther from the reactor face, providing the space to maintain DEMAND as a world-class diffractometer in 10–20 years. By changing the take-off angle of the silicon monochromator, all three incident wavelengths will have a flux increase of a factor of 3–6, and $\lambda/2$ neutron intensity can be significantly reduced using a single PG filter (i.e., choose correct take-off angle for 1.64 Å neutrons). The beam flux at the sample could be a few times higher than the current flux of 2×10^7 n/cm^2/s because more neutrons diffracted by the monochromator could be focused to the sample position. Longer beam space before the sample allows a low-electronic and magnetic field noise environment that is important for the stable high-polarized neutron beam.

HB-1 Polarized Double-Bounce Assembly

The Beam Room Optimization Working Group, formed in response to the HIPAC report, identified possibilities for the HB-1 instrument location to improve performance and the overall space in the beam room. The preferred option was to focus HB-1 on fully polarized diffraction. To realize the potential of such an instrument, a revised HB-1 requires flexibility in polarized beam technology, which could include Heusler, ^{3}He polarizers, or polarizing optics. This upgrade allows tradeoffs between intensity and flipping ratio that cannot be currently realized. Additionally, such an instrument requires adjustable monochromator-to-sample and sample-to-detector distances, which are particularly important for Larmor diffraction measurements. To realize this vision for HB-1, we must replace the monochromator shield assembly. A concept for such a new assembly involves a novel double-bounce monochromator configuration with PG (002) as the first crystal and either PG (002) or Heusler (111) as the second crystal. This concept is possible because of the similar *d*-spacing of these two reflections. Other benefits to this configuration include a fixed sample position for easier space optimization and significantly reduced activation of the Heusler monochromator.

Longer Term Instrument Upgrades

In developing section-level plans, teams identified both near-term and longer-term upgrades. The longer-term upgrades often require significant development effort, including performance simulations and collaboration between NTD and NSD. Examples of such upgrades are described in the following subsections.

CNCS Optics Upgrade

This project involves developing plans and estimating potential performance gains from upgrading and replacing the neutron guides and choppers on CNCS to enable repetition rate multiplication and focusing optics to enable optimization for smaller samples.

SEQUOIA/ARCS Optics Upgrades

The community on the thermal direct geometry instruments typically does not measure large multicrystal arrays, which were commonplace during the planning stages of these spectrometers. This former trend resulted in optics optimized for rather large samples. The incident beam optics on SEQUOIA and ARCS could be redesigned to include the use of focusing devices such as nested mirror optics for increased flux on smaller crystals.

HYSPEC Upgrades of the Bragg Focusing Optics

Varying the horizontal focusing of the incident beam is a method for adjusting the beam profile to fit the dimensions of the sample and the specific requirements of an experiment. Incorporating a Mica monochromator and a focusing polarizer system will enable achieving smaller incident energies and superior energy resolution. This enhancement will broaden the scope of polarization analysis applications across diverse scientific research fields.

NSE Performance

The IAB suggested a "… detailed technical evaluation that includes a complete understanding of the reasons for the disappointing performance of the NSE at the FTS." Careful analysis of the instrument optics and components is required to develop future plans to improve the performance of the NSE instrument at SNS. Additionally, a detailed design of a HFIR-NSE instrument must be performed to understand performance of that instrument and develop a full roadmap for NSE capabilities at ORNL.

BioVSANS

The Bio-SANS instrument is currently able to measure to a lowest accessible Q of 0.001 $Å^{-1}$, corresponding to a largest observable length scale of about 300 nm. Leveraging technology advancements in neutron optics, it has been proposed to increase the spatial range accessible by the Bio-SANS instrument by incorporating three new components: biconcave lenses, right angle prisms, and a high-resolution detector. The purpose of the lenses is to focus the beam to a smaller spot on the detector. The prisms will correct for gravitational effects caused by spread in neutron wavelengths in the beam, and a high-resolution detector will resolve angles finely around the transmitted beam. With the recent upgrade of the collimator vessels, automatic insertion/removal of optical components during operation is now possible. This upgrade will afford access to $Q_{min} \approx 3 \times 10^{-4}$ $Å^{-1}$, benefiting the biological community in the study of complex biosystems.

MAGREF Advanced Focusing Optics

This upgrade will implement a virtual source (VS) together with focusing optics, enabling the use of the full beam divergence for specular reflectivity. The VS is defined by a slit system that can be rotated to allow cutting the beam into a shape that corresponds to the shape of a rectangular sample at small angles. This shaped beam is then projected onto the sample surface through a Selene neutron guide (SNG). The SNG consists of two elliptical neutron guide sections with a reflector at the top/bottom and left/right, respectively. The ellipse refocuses the beam from the VS back to a middle focus, which is distorted by geometrical aberration effects. The second ellipse, by symmetry, corrects for these aberrations, recovering the shape of the VS slit at the sample position. This upgrade will allow the transport of all neutrons that can interact with the sample surface in the experimental cave while removing neutrons that cannot interact with the sample, thereby reducing background and improving the signal-to-noise ratio.

SNAP Beamline Rearrangement

This upgrade will consist of retrofitting the 12 m of under-shielding flight path with neutron guides to increase flux at sample position, adding incident-beam Söller slits in the cave to recover low-divergence beam when needed, redesigning the sample area by adding coverage on one hemisphere with fixed detector enabling unobstructed access to the sample position, and building a downstream station with in-cave guides for low-background microdiffraction/spatially resolved measurements for operando measurements. Overall, this upgrade will improve beamline operations, broaden the scope of science that can be explored, and improve the high-pressure program.

MaNDi Optimize Optics and Incorporate DNP

Redesigned and optimized incident beam optics can provide increased flux on sample and the ability to measure smaller crystals. Following the deployment of DNP on the IMAGINE-X instrument, this capability could be deployed on MaNDi to provide large improvements in the signal-to-noise ratio.

Polarization Strategy

Several instrument teams identified polarized neutrons as an area for potential future growth. Examples include CNCS, BASIS, VERITAS, TOPAZ, NOMAD, POWGEN, and WAND^2. The Polarization Steering Committee is in the process of developing a strategy for polarization development and deployment with prioritization based on opportunities for scientific impact. This strategy will help prioritize future requests for polarization capabilities and better align development efforts in NTD with the scientific needs of the user community. This prioritization must also consider future instruments at STS.

MARS Simultaneous Neutron and X-ray Imaging (SNAX)

Neutron imaging is known to provide unique and complementary contrast compared to X-ray imaging. However, for samples that are evolving with time or undergoing stochastic processes, it is not possible to image with neutrons and X-rays at different locations or facilities. To address this, simultaneous neutron and X-ray systems have been implemented at other world-class neutron facilities and benefiting many research projects for years. For example, ILL implemented this capability in 2016, NIST implemented this capability in 2015 and plans to upgrade in 2022/2023, FRM-II is currently implementing this capability, PSI has used X-rays since 2006 and is planning to upgrade to a simultaneous system. Therefore, a concurrent neutron and X-ray imaging system is proposed to bridge this capability gap. The new x-ray setup will be compatible with the future NB-4 instrument after HBRR.

Potential Second Target Station Instruments

At the time of initial construction of SNS, the site was designed to accommodate an additional target station. The STS project is proposed to fulfill this original vision. The STS project received Critical Decision (CD)-0 approval in 2009, and it was recognized that capabilities more than an order of magnitude beyond the SNS FTS "will close mission capability gaps in nanoscience, biomaterials, energy storage media, structural materials and magnetic systems." The project received CD-1 approval in November 2020, and the facility science mission and impact were described in the *First Experiments Second Target Station Spallation Neutron Source* report, which was issued in January 2020.[4]

The STS project is enabled by the Proton Power Upgrade project, which doubles the SNS accelerator proton power to 2.8 MW. Diverting one out of four pulses allows delivery of 700 kW to STS at 15 Hz and 2.0 MW to FTS (at a frequency of 60 Hz but with 45 pulses per second). The proton beam directed to STS will strike a rotating, segmented, solid tungsten target. Spallation neutrons will be moderated by a series of coupled hydrogen moderators optimized for high brightness. This configuration will result in beams of cold neutrons with the highest brightness in the world, as shown in Figure 19.

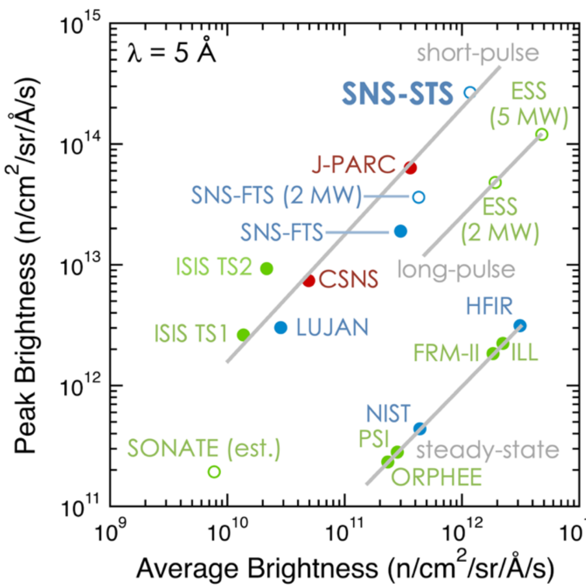

Figure 19. Peak and average brightness of cold neutrons provided by STS compared with other sources.

Possible STS Instrument Suite

A recent Basic Energy Sciences Advisory Committee Facilities Subcommittee report viewed the STS project as "having the potential to be ***absolutely central*** to future world-leading science, with the potential to enable discovery science and technologies, in the fields of quantum materials for computing and sensors, biological and soft materials for science, energy, national security and medicine. The science case must be more fully developed to specify the currently inaccessible grand challenges that the new capabilities can address." This report recommended "STS will be ***ready to proceed*** to CD-2 once the science case is refined and the instrument suite redefined to support the science. Development of the science case is essential." Following this report, a community-led effort to refine the science case was initiated and will be followed by an exercise to reconsider the instrument suite.

For the sake of this document, it is helpful to understand what instruments are possible at STS. Although the eventual instrument suite of STS is yet to be determined, an earlier exercise selected the eight instruments that would be part of the initial suite built during the project. The following eight instruments were selected via a process that completed in July 2021:

BWAVES (Broadband Wide-Angle VElocity Selector spectrometer): An indirect-geometry spectrometer where the final energy of scattered neutrons can be selected or filtered mechanically by a wide-angle velocity selector. This spectrometer features a dynamic range spanning 5 decades, allowing measurements with energy transfers from 10 μeV to ~1000 meV. This dynamic range enables

[4] https://neutrons.ornl.gov/sites/default/files/STS_First_Experiments_Report.pdf

measurements of both vibrational and relaxational excitations simultaneously. BWAVES will be optimized for bioscience, chemical science, and soft matter research. It will be ideal for studying novel materials for energy applications, soft matter such as recyclable polymers, and for better understanding the biological processes in emerging biotechnologies and medical technologies.[5]

CENTAUR: A small- and wide-angle neutron scattering (SANS/WANS) instrument with diffraction and spectroscopic capabilities to simultaneously probe time-resolved atomic- to mesoscale structures in hierarchical systems under in situ or operando conditions. Simultaneous SANS/WANS and diffraction capabilities will be a unique capability among neutron scattering instruments in the United States. It will also provide a direct-geometry spectroscopy option as well as polarized neutrons. CENTAUR will provide needed capabilities in soft matter and polymer sciences, geology, biology, quantum materials, and other materials sciences that need in situ and operando experiments for kinetic and/or out-of-equilibrium studies.[6]

CHESS: A direct-geometry neutron spectrometer with focused beams optimized to detect and analyze weak signals intrinsic to small cross-sections, such as small sample mass, small magnetic moments or neutron absorbing materials. The STS 15 Hz repetition rate will allow use of the repetition rate multiplication technique, expanding the information that can be gained in a single measurement. CHESS will also be designed to employ *XYZ* polarization analysis. The instrument will be optimized to enable studies on quantum materials, spin liquids, thermoelectrics, battery materials, superconductors, and liquids.[7]

CUPI2D (Complex, Unique and Powerful Imaging Instrument for Dynamics): Designed to combine direct and indirect imaging across a broad range of length and time scales. The instrument combines Bragg edge imaging and neutron grating interferometry. CUPI2D is designed for applications that involve length scales from angstroms to micrometers, and timescales from minutes to hours. Leveraging the high flux of cold neutrons from the high-brightness STS cylindrical moderator, CUPI2D permits in situ and operando experiments. Application areas include engineering materials, cementitious materials, nuclear materials, biology and ecosystems, and medical and dental biomaterials.[8]

EXPANSE (EXPanded Angle Neutron Spin Echo): Designed to conduct high-energy resolution studies (nano- to microelectronvolts) of dynamic processes across a broad range of materials. The wide-angle detectors will provide a coverage of nearly two orders of magnitude in scattering wavevector and approximately four orders of magnitude in Fourier times. Additionally, EXPANSE be equipped with a fast chopper near the sample to function as a direct-geometry chopper spectrometer with polarized neutrons. In this mode, the magnetic field will be turned off and time-of-flight analysis will be used to

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[5] E. Mamontov et al. “A concept of a broadband inverted geometry spectrometer for the Second Target Station at the Spallation Neutron Source.” *Rev. Sci. Instrum.* **93**, 045101 (2022).
[6] S. Qian et al. “CENTAUR—The small- and wide-angle neutron scattering diffractometer / spectrometer for the Second Target Station of the Spallation Neutron Source.” *Rev. Sci. Instrum.* **93**, 075104 (2022).
[7] G. Sala, et al. “CHESS: The future direct geometry spectrometer at the second target station.” *Rev. Sci. Instrum.* **93**, 065109 (2022).
[8] A. Brügger et al. “The Complex, Unique and Powerful Imaging Instrument for Dynamics (CUPI2D) at the Spallation Neutron Source.” *Rev. Sci. Instrum.* **94**, 051301 (2023).

expand the energy window offered by the NSE mode (standard operation mode) by two orders of magnitude on the high-energy transfer side in the range of micro- to millielectronvolts while providing approximately one order of magnitude overlapping time range. Application areas include energy materials, soft matter, liquids and glasses, quantum materials, engineering materials, and biological materials.[9]

PIONEER: A time-of-flight, single-crystal diffractometer optimized for studying small-volume samples (<1 mm^3) in a range of sample environments. The instrument will reduce sample volume requirements for single-crystal neutron diffraction by more than one order of magnitude, allowing detailed atomic-scale structural characterization of materials at the earliest stages of discovery. PIONEER will be capable of measuring tiny crystals (~0.001 mm^3) and thin epitaxial films (~10 nm thicknesses × 25 mm^2 area). It will also provide a polarized beams for studying weak magnetic scattering signals and will possess a high-resolution mode to probe large unit cells up to 200 Å. With a 4 Å wavelength band and 4.4 sr detector coverage, PIONEER will measure a broad reciprocal space at a single sample position. Applications include quantum materials, energy related materials, thin films and heterostructures, planetary science, and mineral physics and will enable time-resolved studies across these scientific areas.[10]

QIKR: A general-purpose, horizontal-sample-surface reflectometer consisting of two independently operable end stations—one with the incident beam directed up and one directed down. It will collect specular and off-specular reflectivity data faster than any other such instrument. Using pulse skipping (7.5 Hz), it will often be possible to collect complete specular reflectivity curves using a single instrument setting to provide cinematic operation, in which the user records the sample undergoing time-dependent modification with frame rates as fast as 1.0 Hz. Cinematic operation will be deployed to observe such processes in real time as in situ polymer diffusion and reaction, battery electrode charge–discharge cycles, hysteretic phenomena, membrane protein insertion into lipid layers, and lipid flip-flop.[11]

VERDI (VERsatile DIffractomter): A wide-bandwidth diffractometer with full polarization capability for powder and single-crystal samples. The instrument will offer high resolution at low momentum transfers and excellent signal-to-noise for routine measurements of small magnetic-moment compounds, milligram-size samples, diffuse magnetic signals, and large unit cell organic compounds. Optics design will provide flexibility in beam divergence, providing a high-resolution powder mode, a high-intensity single crystal mode, or a polarized beam option. VERDI will be equipped with a wide-angle supermirror analyzer for automated transition between unpolarized, half-polarized, and linear *XYZ* polarization analysis options. The anticipated core user community will be involved in studies of energy materials and quantum magnetism where VERDI will enable the ability to probe spin behaviors that are inaccessible using other techniques. Additionally, the implementation of polarization allows the isolation of not only

[9] C. Do et al. “EXPANSE: A time-of-flight EXPanded Angle Neutron Spin Echo spectrometer at the Second Target Station of the Spallation Neutron Source.” *Rev. Sci. Instrum.* **93**, 075107 (2022).
[10] Y. Liu et al. “PIONEER, a high-resolution single-crystal polarized neutron diffractometer.” *Rev. Sci. Instrum.* **93**, 073901 (2022).
[11] J. F. Ankner et al. “Cinematic reflectometry using QIKR, the quite intense kinetics reflectometer.” *Rev. Sci. Instrum.* **94**, 013302 (2023).

magnetic scattering but also incoherent scattering, which offers clear advantages for studying nonmagnetic hydrogen-based materials.[12]

In the process of selecting these eight instruments, four other concepts were considered:

M-STAR: A next-generation polarized reflectometer capable of performing measurements at one setting in a broad range of Q up to 0.3 Å^{-1} for specular, off-specular, and GISANS measurements. M-STAR will be optimized for nanoscience and spintronics studies on small samples (~2 mm × 2 mm). Science areas include novel quantum materials, topological insulator heterostructures, functional materials, and nonequilibrium properties.[13]

MENUS: A high-flux, versatile, multiscale materials engineering diffraction beamline, providing integrated diffraction, SANS, and imaging capabilities. MENUS will provide crystallographic and microstructure data to elucidate lattice strain, phase transition, microstructure, and texture evolution in three orthogonal directions in complex material systems under extreme applied conditions.[14]

EWALD: A next-generation neutron macromolecular crystallography beamline. EWALD will be a single-crystal diffractometer capable of collecting data from macromolecular crystals orders of magnitude smaller than what is currently feasible and will enable key discoveries in the biological, biomedical, and bioenergy sciences.[15]

TITAN: A multimodal beamline enabling diffraction, spectroscopy, and SANS in applied magnetic fields above 20 T. It will provide a platform for deployment of 20–25 T vertical split-core magnets based on high-temperature superconducting conductor technology. TITAN will be compatible with dilution temperatures and moderate-pressure diamond anvil cells, allowing for coupled extremes measurements on quantum materials.[16]

Other ideas could include the following:

ZEEMANS: Platform to enable multimodal neutron scattering in a horizontal field magnet. The High Field Magnet of Helmholtz-Zentrum Berlin is being transferred to SNS. This magnet, coupled with a high-temperature superconducting insert, could enable neutron scattering in fields exceeding 30 T. This instrument will combine the highest fields possible at any scattering facility with the world's brightest source of cold neutrons.

Q-MIGS (Quantum Materials Indirect Geometry Spectrometer): Instrument utilizing the white beam spectrum of STS together with a multianalyzer secondary spectrometer. The broad bandwidth and high brightness of STS, combined with a secondary spectrometer capable of measuring a continuous band of

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[12] V. O. Garlea et al. "VERDI: VERsatile Diffractometer with wide-angle polarization analysis for magnetic structure studies in powders and single crystals." *Rev. Sci. Instrum.* **93**, 065103 (2022).
[13] V. Lauter et al. "M-STAR Magnetism second target advanced reflectometer at the Spallation Neutron Source." *Rev. Sci. Instrum.* **93**, 103903 (2022).
[14] K. An et al. "MENUS—materials engineering by neutron scattering." *Rev. Sci. Instrum.* **93**, 053911 (2022).
[15] G. E. O. Borgstahl et al. "EWALD: A macromolecular diffractometer for the second target station." *Rev. Sci. Instrum.* **93**, 064103 (2022).
[16] B. L. Winn et al. "A flexible neutron spectrometer concept with a new ultra-high field steady-state vertical-bore magnet." *Rev. Sci. Instrum.* **93**, 123903 (2022).

final energies, can enable inelastic neutron scattering on significantly smaller crystals than can be measured with any current or proposed instrument in the world. This capability could open the door to neutron spectroscopy studies on artificial heterostructures and can be compatible with high-temperature superconducting vertical field magnets. Coupling this instrument with polarizing supermirrors could enable fully polarized measurements of $S_{\alpha\beta}(\mathbf{Q},\omega)$.

HERTZ (High Energy Resolution Terahertz Spectrometer): An additional direct-geometry spectrometer that would serve as a higher-resolution complement to CHESS. The principal difference between CHESS and HERTZ is the longer sample-to-detector distance of the latter, resulting in better resolution. Cold neutron direct-geometry spectrometers at SNS are highly oversubscribed, and performance gains of more than an order of magnitude on STS call for multiple instruments to meet community demand and to address the most complex and impactful scientific problems.

BER-SANS**:** A mirror focusing optics SANS beamline at STS with focal spot at the sample will provide complementary capabilities for studying small sample volumes of dilute bio-macromolecular solutions in kinetic measurements. A DOE BER-funded concept study has been published.[17]

SANS-1**:** SANS instrument for the real-time study of how atomic structures form in complex materials. This SANS instrument will provide new opportunities for the study of time-resolved phenomena and kinetics associated with processing, 3D printing, or the assembly of complex polymers, soft materials, nanomaterials, and quantum materials. SANS-1 is a general-purpose instrument with excellent detector coverage that makes the best use of the high flux provided by STS. A proposed inclusion of a statistical chopper for discriminating elastic from inelastic scattering would be unique among SANS instruments.

VBPR (Variable Beam Profile Reflectometer): A variable-beam profile reflectometer with an elliptical guide system will focus a divergent beam, allowing its profile, or footprint on the sample, to be tuned, thus optimizing illumination of small samples. The beam profile on sample is expected to range from ~1 mm^2 to several hundred square millimeters.[18]

Wide-Bandwidth Disordered Materials Diffractometer: This total scattering instrument would enable the simultaneous determination of interatomic to mesoscopic structures. In some ways, this capability would be technically similar to the CENTAUR concept but built from the point of view of a wide-angle powder diffractometer rather than a SANS instrument. This results in diffraction capabilities with better Q resolution but SANS capabilities with a higher Q_{min}, similar to the NIMROD instrument at the ISIS Neutron and Muon Source. This instrument would enable detailed structural measurements of large porous systems such and zeolites and metal–organic frameworks and the interaction of liquid and gases within their frameworks for applications such as catalysis, gas storage and separation, and fuel cell development.

[17] C. U. Wildgruber et al. "A Science Driven Approach to Optimize the Conceptual Design for a Biological Small-Angle Neutron Scattering Instrument." *J. Appl. Crystallogr.* **57**, 818 (2024).
[18] J. Stahn, U. Filges, and T. Panzner. "Focusing specular neutron reflectometry for small samples." *Eur. Phys. J.-Appl. Phys.* **58**, 11001 (2012).

Impact on SNS and HFIR Instruments

Although the instruments described above are notional, the list and descriptions show instrument types that are ideally suited to STS. The following section describes the long-term considerations for instruments at SNS FTS and HFIR.

Spectroscopy

The current suite of spectrometers at SNS and HFIR comprise four triple-axis spectrometers, four direct-geometry spectrometers, two indirect-geometry spectrometers, and one NSE instrument. Of this suite, the triple-axis spectrometers are optimized for high-flux in a more restricted range of **Q**,ω and, as such, will remain complementary after completion of STS. Because STS is focused on cold neutrons, the two thermal direct-geometry instruments (ARCS and SEQUOIA) and the thermal indirect-geometry spectrometer (VISION) will remain world leading. The main instruments of consideration are the two cold neutron direct-geometry spectrometers (CNCS and HYSPEC) and the NSE spectrometer, because they view a coupled hydrogen moderator at SNS FTS. The BASIS backscattering spectrometer views a high-resolution decoupled hydrogen moderator (not available at STS) and will continue featuring the highest energy resolution for measurements in the energy domain even after the completion of the STS instruments.

For SNS-NSE, the capabilities are certainly distinct from the proposed EXPANSE instrument. However, these differences call for a strategy for NSE that incorporates the current SNS-NSE and future instruments at STS and HFIR. An unfortunate complication in this discussion is the uncertain future of NCNR. NCNR was in the process of building a new spin echo instrument funded by NSF when their reactor issues occurred. If NCNR is restored to full 20 MW operation, then the national landscape for NSE capabilities will change significantly. Another open question is the possibility of resonant spin echo techniques as an alternate manner of obtaining similar information.

The two cold neutron direct-geometry spectrometers, CNCS and HYSPEC, are in high demand from the user community. CNCS is our workhorse cold neutron direct-geometry spectrometer. The quantum materials demand for this instrument is sufficiently high that the CHESS instrument alone will not meet the community demand. However, once CHESS and HERTZ are both constructed, the situation may be different. Most cold neutron direct-geometry spectrometers internationally have an active program in quasielastic neutron scattering (QENS) studies. Such measurements are performed on CNCS and provide a lower resolution, but broader dynamic range compared with BASIS. However, the beamtime available for QENS in CNCS is small because of the high demand from the quantum materials community. Shifting most quantum materials cold neutron spectroscopy measurements to STS will enable a shift of the CNCS science program toward QENS studies, enhancing the chemical spectroscopy suite.

HYSPEC is a unique instrument that provides access to full polarization analysis on a direct-geometry spectrometer. This instrument has played an important role for developing the technique and building the user community that employs polarized time-of-flight spectroscopy. The CHESS instrument is designed to be fully polarized. However, the use of polarized ^{3}He neutron spin filters for analyzing scattering polarization limits its applicability to uniaxial polarization studies in low magnetic fields. Consequently, it may be beneficial to consider relocating or reoptimizing HYSPEC to STS or proposing a similar instrument concept in which polarization analysis is conducted using wide-angle supermirror analyzers (this capability could be incorporated into Q-MIGS). The supermirror analyzer offers full flexibility in instrument operation, allowing rapid interchange between polarized and unpolarized modes, and increased tolerance to external magnetic fields produced by vertical- or horizontal-field magnets. Performing polarized inelastic neutron studies in high magnetic fields is a unique and highly demanded capability provided by HYSPEC, which must remain available to the user community. Additionally, HYSPEC's configurability is ideal for prototyping advanced polarization techniques, such as spherical neutron polarization. Additionally, HYSPEC features open access to the sample position, similar to triple-axis spectrometers and in contrast to both current (CNCS) and future (CHESS, HERTZ) cold neutron direct-geometry spectrometers, uniquely allowing for placement of bulky external probes near the sample position that cannot be accommodated at other SNS spectrometers.

Diffraction

The current suite of diffractometers at HFIR and SNS consists of nine diffractometers: two time-of-flight powder diffractometers (NOMAD and POWGEN), a constant-wavelength powder diffractometer (MIDAS), a constant-wavelength powder and single-crystal diffractometer ($WAND^2$), a constant-wavelength single-crystal instrument (DEMAND), two time-of-flight single-crystal instruments (TOPAZ and CORELLI), and two macromolecular crystallography instruments, (MaNDi and IMAGINE). The powder diffraction suite at FTS would be completed with the construction of the DISCOVER beamline and possibly a HighResPD instrument.

The two time-of-flight powder diffractometers (NOMAD and POWGEN) are in high demand and would still be in high demand once DISCOVER is available. Together, these instruments will provide high-flux measurements, in situ details, structural measurements, and high-resolution measurements using the medium- to short-wavelength neutrons that are provided by FTS. These instruments would be complemented by the STS VERDI instrument, which would be able to study magnetic and nuclear structure of systems with large unit cells using the high flux of longer wavelength neutrons of STS in addition to the unique polarization capabilities it will bring.

In a similar way, the current time-of-flight single-crystal instruments TOPAZ and CORELLI use the medium-to short-wavelength neutrons of FTS. TOPAZ will remain the instrument of choice for detailed structural measurements of single crystals. CORELLI, with its large detector array and unique correlation chopper capabilities, will remain in high demand for the study of magnetic and nuclear structure of order and disorder in crystalline materials. These instruments will be complemented by the high flux of polarized long-wavelength neutrons available on the STS PIONEER instrument, which will enable detailed magnetic structural studies of smaller crystals.

The constant-wavelength diffractometers at HFIR (MIDAS, $WAND^2$ and DEMAND) are in high demand, particularly where their ability to more easily access complex sample environments is needed. The need for this complimentary capability will remain even after diffractometers, such as VERDI and PIONEER, come online at STS. With the construction of EWALD at STS, three macromolecular diffractometers will be available. The IMAGINE-X instrument integrates the DNP technique, which will dramatically improve the signal-to-noise ratio of neutron diffraction data and greatly enhance the sensitivity of neutron macromolecular crystallography. A strategic plan will be developed to describe how these instruments will be utilized by the biology community, the foreseen demand, and needs for the next 10 years and beyond. This plan may determine that there is a clear need for all three instruments in their current configuration, whether instrument upgrades and modifications are needed, and possibly areas where one or more of the instruments could diversify their science program.

Large Scale Structures

The Large-Scale Structures (LSS) suite of 11 instruments at SNS and HFIR comprises a diverse set of techniques. The instruments are in high demand and consistently oversubscribed by general user proposals. The suite includes two neutron imaging instruments: MARS at HFIR and VENUS at SNS. Small-angle scattering instruments in the suite include two velocity-selector, pin-hole SANS instruments at HFIR (GP-SANS and Bio-SANS) along with the time-of-flight EQ-SANS and a Bonse–Hart type crystal monochromator USANS at SNS. The suite operates a horizontal geometry liquids reflectometer (LIQREF) and a polarized beam magnetism reflectometer (MAGREF), both at SNS. The LSS suite of instruments also includes specialized diffractometers for engineering materials (HIDRA at HFIR and VULCAN at SNS) and for high pressure/extreme environment studies (SNAP at SNS). The low angle/fine energy resolution SNS-NSE spectrometer is organizationally grouped with the SANS instruments in the LSS section; however, in the present context, it is discussed with other spectrometers in the spectroscopy sections of this document.

The present instruments of the LSS suite will retain world-class status and continue to provide many unique technical capabilities, while the SNS STS will provide new opportunities with brighter beams suited for measuring smaller samples and performing faster kinetic experiments over a wide Q range. The focus of the SNS STS on long wavelength and high brightness will further enhance the techniques of the LSS suite.

Among the currently proposed set of eight first STS beamlines is the SANS/WANS instrument CENTAUR, which will provide an extremely wide simultaneous Q range and high brightness, which are excellent for in situ studies on small sample volumes. Meanwhile, GP-SANS upgrades for polarized beam capability, picture frame multidetector arrays, focusing beam at the detector position, and high-resolution low-Q detector will keep the GP-SANS instrument at HFIR world leading, with high integrated beam intensity and low background, to reach the lowest SANS Q values with excellent flux. Similarly, Bio-SANS at HFIR will focus its mission on very small Q values and a wide dynamic range, fitting a mission space on complex hierarchical biomaterials, such as plant tissues. The addition of lenses and prisms will reduce the minimum Q by more than a factor of 3 (BioVSANS). A focusing-optics SANS beamline (BER-SANS) at STS with focal spot at the sample will provide complementary capabilities for studying small sample volumes of dilute bio-macromolecular solutions in kinetic measurements. The EQ-SANS instrument at FTS will retain its excellent $\Delta Q/Q$ resolution, providing a superb capability for the important field of membrane diffraction, and its chopper upgrade will offer a unique monochromatic option for the study of samples with high incoherent background. Competitiveness of all SANS instruments requires continuous development of sample environment capabilities. Sample environment transferability between CENTAUR and EQ-SANS will facilitate optimal use of the entire suite of SANS instruments.

The current reflectometry suite includes two instruments, MAGREF and LIQREF at FTS. They share a common primary shutter and guide assembly before the optics split the neutrons to provide a downward sloping beam to LIQREF and a flat beam to MAGREF. On STS, the QIKR, M-STAR, and VBPR (Variable Beam Profile Reflectometer) instruments will serve similar science communities while being optimized for the larger wavelength band and smaller moderators offered by STS. A single instrument setting on the STS reflectometers would require several instrument settings on the FTS reflectometers to cover the same Q space measurement envelope. Any experiment that can make use of this large measurement envelope will benefit from using an STS instrument. For cases in which the features of interest are in a narrow band of Q space, the current FTS instruments will remain world leading, assuming gains are made through neutron optics upgrades.

Current instruments for measuring engineering materials at SNS FTS and HFIR are VULCAN and HIDRA, respectively. HIDRA is a monochromatic instrument that focuses on high spatial resolution measurements of single-peak-based residual strain/stress. VULCAN is a versatile time-of-flight diffractometer that is focused on in situ/operando studies of engineering materials under complex external stimuli. These two instruments complement each other, particularly in residual stress measurements across wide range of spatial resolution and complexity of engineering material characteristics such as phase and microstructure. The proposed MICRON instrument at FTS views the same type of moderator as VULCAN, with more detector angular coverage while being compact. MICRON fills a capability gap by enabling rapid investigation of material microstructure anisotropy owing to phase and texture in a broad range of engineering and geological materials. At STS, a next-generation engineering material diffractometer MENUS is conceptualized with multimodal operations enabled by a unique detector coverage, including diffraction, SANS, and imaging. This instrument will be tailored for complex engineering materials systems with low symmetry and more constituents. It allows for unprecedented multiple length-scale investigations of complex engineering materials under in situ and operando stimuli by simultaneously probing tensorial lattice strain/stress and crystallographic and morphological material characteristics. The high cold neutron flux provided by STS enables MENUS to extend and complement VULCAN'S capabilities. This family of four engineering diffractometers will constitute the strongest materials and engineering diffraction capabilities in the world.

The CUPI2D imaging instrument at STS will excel with capabilities of grating interferometry, reaching capabilities of an instrument that could truly be termed a neutron microscope. Meanwhile, the MARS instrument at HFIR continues a mission with high overall neutron beam power for leadership in neutron radiography and tomography, and the VENUS beamline at the SNS FTS complements these beamlines with a mission focused on Bragg edge and resonance contrast imaging.

Instruments Enabled by Potential New Guide Halls at HFIR

The PVR project at HFIR can enable the addition of new guide halls at HFIR. Although these discussions are still in the preliminary stage, a likely scenario seems to be inclusion of a thermal guide hall from HB-2 and the cold guide hall at HB-3.

This section describes a possible list of new instruments that could be accommodated at these new HFIR guide halls. With addition of guide halls on HB-2 and HB-3, only one open port will remain in the beam room on HB-1. This list of instruments has not been socialized with the user community or prioritized in any way. It is provided to articulate what may be possible in the future at HFIR.

HFIR Beam Room

HB-1 Hybrid Instrument for Nuclear Energy Applications

Although neutron scattering provides important information on nuclear energy related systems, this community is challenging to serve on existing instruments because of neighboring instruments and the presence of many users and other scientists in the vicinity. A single remaining port in the beam room, provides an opportunity to develop an instrument that would be optimized for this community in a more isolated environment. A hybrid neutron diffraction/SANS instrument for nuclear energy applications could meet many of the needs for such research projects. This instrument would offer benefits such as convenience of transfer from HFIR irradiation experiments, hot-cell preparation labs, and ORNL infrastructure for handling radioactive samples. A preliminary design concept suggests that this instrument could provide SANS capabilities with a Q range of 0.008–0.8 $Å^{-1}$ and diffraction using 1.15 Å neutrons, giving a Q range of 0.82–10 $Å^{-1}$. Specific use cases could include structural characterization of fuel, cladding, structural materials, waste forms, and thermal transport and fuel reprocessing systems, including measurements on highly irradiated samples.

Current Cold Guide Hall (HB-4)

The instrument suite in the current cold guide hall has been discussed and optimized in consultation with the user community and external advisory committees. As such, for the sake of describing a potential future HFIR instrument suite, the assumption is being made that these instruments will remain important and relevant. The instruments listed for the HFIR Guide Hall (HB-4) on Figure 20 represent the plans following the HBRR activity and completion of associated AIPs for MANTA and MARS. This figure also assumes that the MANTA multianalyzer secondary spectrometer is completed, a new NSE spectrometer on NB-2 will be funded and installed, and that USANS will be relocated to NB-2B. These instruments are described in previous sections of this document.

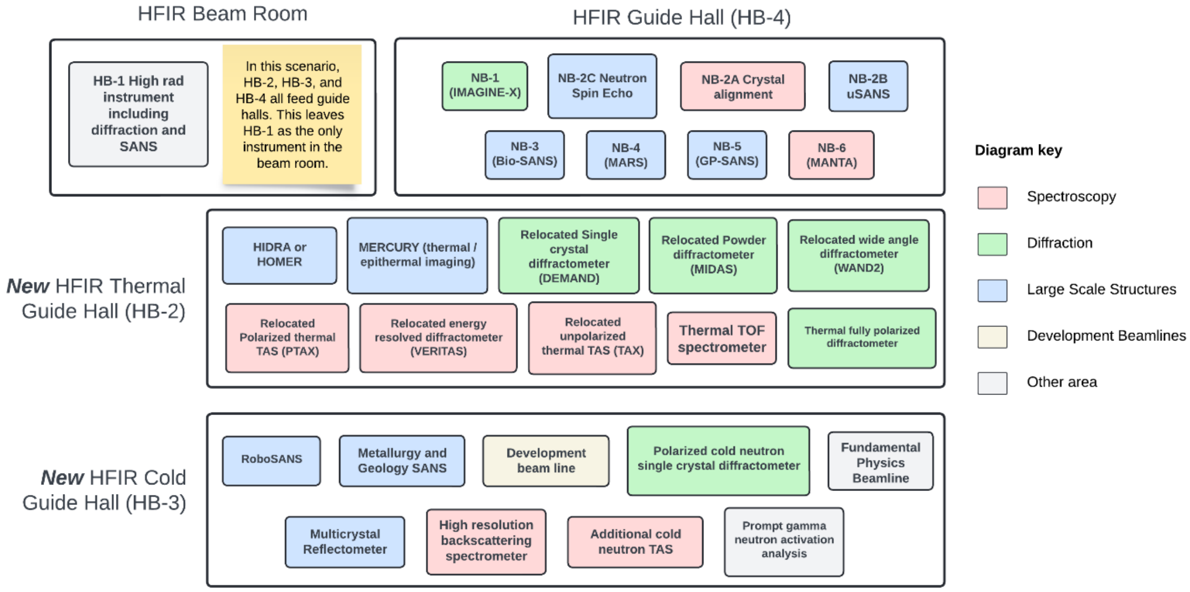


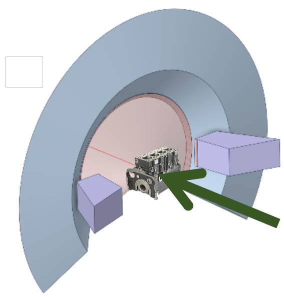
Figure 20. Diagram showing possibilities for future instruments at HFIR with addition of two new guide halls, thermal and cold.

New Thermal Guide Hall (HB-2)

HB-2 provides a world-leading thermal neutron flux owing to its radial view of the HFIR reactor fuel. The radial nature of the beam tube makes installation of a cold source challenging, but this capability will be considered as plans evolve. A thermal guide hall is conceptually simpler on HB-2, but the larger beam tube could also accommodate a large suite of cold neutron instruments. This optimization needs to take place in consultation with the user community, but the possibility of a cold source on HB-2 should be considered carefully because we anticipate larger demand for cold neutron instrumentation, which is best accommodated at HB-2.

The following subsections describe thermal neutron instruments, some of which are relocated and significantly upgraded instruments from the current HFIR beam room and some of which are new concepts. For relocated instruments, the possible new capabilities that can be realized are explained.

HOMER



HOMER (illustrated at left) is an innovative instrument concept developed during the 2020 instrument-building school exercise. It is unlike any other strain-scanning instrument in the world, designed to supplant and significantly enhance the capabilities of HIDRA at HFIR.

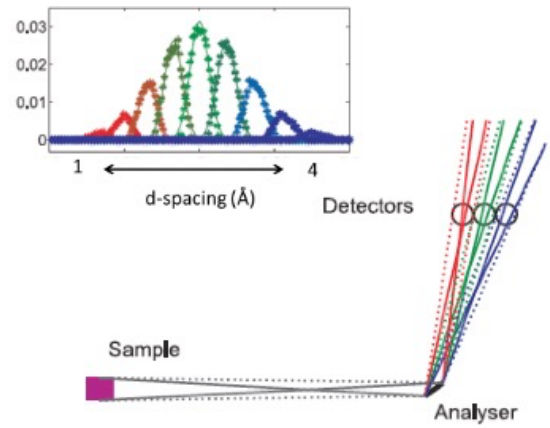


Figure 21. Diagram showing how the white beam analyzers work to achieve a large range of d for any individual ADP.

HOMER can only be accommodated in a thermal guide hall because it requires a white incident beam of neutrons. These neutrons scatter from the sample and are analyzed post-sample to determine diffraction peaks, using an array of analyzer crystals. Figure 21 illustrates how an analyzer/detector pair (ADP) selects a specific range of *d*-spacing at a given scattering vector, resulting from the incident beam interacting with a series of analyzer crystals (PG in the case of HOMER).

Each ADP can measure a strain direction that coincides with the scattering vector, *Q* (Figure 22). Figure 22 shows ADPs set at both 90° 2θ and 70° 2θ in-plane with the sample. Unlike HIDRA, HOMER does not require a focusing monochromator for wavelength determination, allowing detectors to be placed in-plane on either side, producing results similar to VULCAN but with a higher continuous flux than SNS can provide. One of HOMER's key advantages is its ability to interrogate multiple strain components simultaneously, because ADPs can be positioned around the sample area—even out of the plane. Figure 22c shows a map of possible detector placements around the sample area. Placing two ADPs in-plane at ±90° 2θ allows for in situ measurements across a large *Q* range with high data throughput. With a ring mounted at 70° 2θ, a full strain tensor can be measured in a single operation, eliminating the need for sample rotation for tensor analysis. The incident wavelength spectra should range from 1.4 Å to 3.0 Å, targeting engineering materials of interest and making HOMER ideal for HFIR's thermal guide hall.

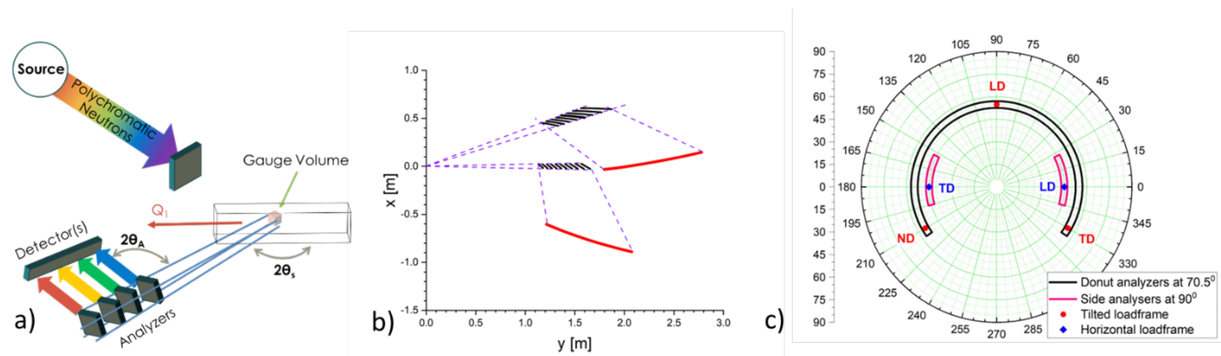


Figure 22. (a) Sketch of example ADP with a sample to illustrate how one pair can obtain one direction of strain along Q. (b) Geometry of the PG analyzers to detectors to achieve a d-range of about 3 Å. (c) Map of optimal locations for full strain tensor determination.

The scientific applications of HOMER closely align with those of HIDRA. Data from diffraction can provide insights into residual stress/strain, phase, and crystallographic texture. Mapping applications include materials joining (such as welding, brazing, friction stir welding, and riveting), heat-treated samples, forgings, extrusions, bearings, races, fasteners, transportation and aerospace components, pressure vessels, piping, nuclear engineering components, and the growing field of AM of metal components. In advanced manufacturing processes such as fusion powder bed AM, direct energy deposition, and additive friction stir deposition, mapping full-strain tensors is crucial for understanding residual shear strain. HOMER will also benefit research on functional materials in varied environments, such as piezoelectric materials in applied fields and shape-memory alloys under varying load and temperature conditions. With the ability to measure full tensors without remounting and HFIR's superior continuous flux, HOMER will enable advanced in situ and operando characterization of complex materials and processes (e.g., welding, AM, thermal treatment, forging). Challenges in materials joining, such as stress relaxation cracking and microstructural evolution at high heating rates (~10–30 °C/s), can be addressed using equipment such as Gleebles.

The combination of flux and *Q* range at HOMER will provide unparalleled capabilities, unmatched by any reactor-based instrument worldwide. These advancements are critical for upcoming in situ and operando studies, which are essential for the progression of materials science in the coming decades.

MERCURY

One proposed scientific enhancement is the creation of an epithermal and fast neutron radiography station on a thermal beamline at HFIR with the ability to image highly radioactive specimens such as irradiated nuclear fuel rods, isotope production targets, or spallation neutron target materials. Performing radiography and tomography on such materials with thicknesses of more than a few millimeters would prove to be challenging with thermal or cold neutrons. Furthermore, these types of materials have likely already been processed, irradiated, and tested at ORNL. Having a facility (MERCURY at HFIR and VENUS at SNS) near the handling areas designated for highly activated materials would simplify transportation and would enable quick determination of irradiation effects for a variety of materials. The HFIR Beam Room Optimization Working Group concluded that "there isn't space in the HFIR beam room for such an instrument … this concept would be more appropriate when there is a thermal guide hall at HFIR due to the size and operational complexity of such an instrument."

Relocated Single-Crystal Diffractometer

The HB-3A (DEMAND) single-crystal neutron diffractometer is currently a versatile, high-throughput instrument with multiple modes, including two-axis and four-circle configurations to accommodate various sample environments, and options for polarized and unpolarized neutron beams to explore novel magnetism and structures. However, it shares a beam port with the HB-3 triple-axis spectrometer, which limits the choice of monochromators and results in a high background. Relocating the instrument to the thermal guide hall would significantly enhance beam performance and reduce background noise. Additionally, the expanded space would allow for the use of more extreme sample environment equipment at the beamline, which is critical for advancing research in condensed matter physics.

Relocated Powder Diffractometer

The upgraded HB-2A (MIDAS) powder diffractometer will be a high-throughput instrument ideally suited for studying new, complex, magnetically ordered systems. HB-2A accommodates experiments requiring complex and extreme sample environments, and improved counting times will enable in situ type measurements. However, the limited space in the beam room and proximity to nearby instruments hinders the use of more extreme sample environments and results in a higher background. Relocating the instrument to the thermal guide hall would allow higher magnetic fields, improved polarization capabilities (lower stray fields), and lower background. The expanded space would also enable full detector coverage and higher resolution, as well as the possibility for different monochromators and takeoff angles to tune the wavelength and resolution to the specific experiment.

Relocated Wide-Angle Diffractometer

WAND² is a versatile powder and single crystal diffractometer that supports a diverse scientific user community. To improve this versatility, WAND² would strongly benefit from a position on a thermal guide using a monochromator drum to access multiple wavelengths of a diamond monochromator. A telescoped sample table and additional monochromator takeoff angles allows for optimized monochromator-to-sample distance and, ultimately, instrument resolution. This concept has been developed as part of the instrument building workshop in 2021. The overall lower background of a thermal guide hall could improve the signal-to-noise ratio, especially necessary for extremely small samples commonly explored on WAND². The expanded space also enables extreme and in situ sample environments (e.g. laser excitation, levitator experiments, super high field, chemical reaction cell).

Relocated Polarized Thermal Triple-Axis Spectrometer

The HB-1 (PTAX) thermal triple-axis spectrometer is used to perform polarization analysis of elastic and inelastic scattering. Relocation to a guide hall would benefit the instrument performance in several ways. The biggest impact would be the installation of a *tanzboden*, or dance floor, and the use of airpads to easily change the distances between monochromator and sample and sample and analyzer. This configuration can provide better *d*-spacing resolution for Larmor diffraction, better energy resolution for inelastic spin echo, and expanded sample environment space for spherical neutron polarimetry. Nonmagnetic materials will be used for the monochromator shield and the secondary spectrometer, improving neutron polarization of the incident and scattered beams. A horizontal field cryomagnet, which cannot be used in the beam room because magnetic materials surround the sample area, could be used here, expanding polarization capabilities. Incorporation of a velocity selector and the reduced transmission of high-energy neutrons from the thermal guide would suppress the activation of the Heusler monochromator and would also reduce the neutron background. The relocation provides an opportunity to separate the polarized thermal triple-axis spectrometer from other instruments that use cryomagnets because fringe fields affect the performance of the Wollaston prisms and spherical neutron polarimetry apparatus. Combining these optimizations with the thermal flux from HB-2 would produce an instrument competitive with the best in the world.

Relocated Unpolarized Thermal Triple-Axis Spectrometer

The HB-3 (TAX) spectrometer is currently the workhorse unpolarized thermal triple-axis spectrometer. The physical constraints of the beam room significantly limit the functionality of this spectrometer compared with international competition. Relocation to a thermal guide hall would enable development of an optimized monochromator changer, the inclusion of a tanzboden to enable movements of the sample position and analyzer assembly on airpads, and the ability to incorporate double focusing optics. A monochromator changer will enable switching between up to four monochromator assemblies while maintaining low background. Double-focusing optics will enable flux increases (of about 3×), and the inclusion of a virtual source and monochromator in a Rowland circle geometry can further reduce background. The tanzboden will enable exchanges of secondary spectrometers with one assembly optimized for high signal to noise at a restricted range of $\mathbf{Q},\omega$ space, while a second assembly could be optimized for broader surveys within a $\mathbf{Q},\omega$ plane of scattering. Combining these capabilities with the flux on HB-2 would certainly produce an instrument competitive with the best in the world.

Relocated Energy-Resolved Diffractometer

The HB-1A (VERITAS) fixed incident energy (E_i = 14.5 meV) triple-axis spectrometer is mostly used for parametric studies of magnetic and structural phase transitions in materials. It is an excellent instrument for measuring weak magnetic signals from small single-crystal and thin-film samples under a wide range of complex sample environments, including a four-circle goniometer and small 2D detector option. The HB-1A location in the existing thermal beam room applies significant constraints that prevent full optimization of HB-1A. Relocating to the new thermal guide hall will benefit the performance and greatly enhances the flexibility of HB-1A: (1) HB-1A does not have its own beam tube and operates at fixed wavelength of λ = 2.38 Å by utilizing a double-bounce monochromator system; relocating to the new guide hall will provide opportunity to optimize the incident beam optics (e.g., multiple wavelengths which are ideal for a diffractometer); (2) allow more space between monochromator–sample and sample–analyzer, which are critical distances for expanding/accommodating sample environment capabilities (e.g., high vertical and horizontal magnetic field) and for fully optimizing neutron polarization capabilities with a high flipping ratio; and (3) enable lifting counter of the backend. Combining these improvements with the flux on HB-2 will produce an energy-resolved diffractometer with high flux, high signal-to-noise ratio, and high flexibility to complement the suite of diffractometers at ORNL.

Thermal Time-of-Flight Spectrometer

The thermal time-of-flight spectrometers at SNS, BL-17 (SEQUOIA) and BL-18 (ARCS), are world-leading spectrometers that are in high demand from the user community. No appropriate beam ports remain open at SNS FTS to expand these capabilities, and SNS STS is focused on cold neutrons. A new thermal guide hall at HFIR provides a means to expand the capacity for thermal time-of-flight spectroscopy and can be optimized in a complementary manner. One advantage of a reactor-based time-of-flight spectrometer is the ability to optimize the repetition rate for a specific experiment as the frequency is not limited by the pulse rate of the source. Such an instrument would have a more limited range of incident energies than the instruments at SNS, likely limited to a maximum of about 80 meV depending on guide optimization (SNS instruments can utilize neutrons with energies exceeding 2 eV).

Thermal Fully Polarized Diffractometer

Monochromatic beams of neutrons at continuous sources are ideally suited to applications of polarized neutrons. Some techniques benefit from high flux of cold neutrons, whereas others require thermal neutrons. Thermal neutrons are required for measurements of magnetic form factors and for Larmor diffraction, for which obtaining high-resolution measurements of short *d*-spacing reflections is desirable. A fully polarized diffractometer should enable multiple methods of polarization analysis, including ^{3}He polarizers and polarizing monochromators. It should also enable measurements over a wide range of incident energies and with variable distances to enable advanced methods such as Wollaston prisms to achieve a *d*-spacing resolution of $\Delta d/d \approx 10^{-6}$. This instrument will also be compatible with the recently developed spherical neutron polarimetry device for complete mapping of the polarization tensor.

New Cold Guide Hall (HB-3)

Addition of a new cold guide hall could provide an opportunity to add unique capabilities or expanded capacity to the US neutron scattering community. Some examples of what could be included are listed in the following subsections.

RoboSANS

This instrument would be designed as a medium-flux, medium-resolution SANS beamline, which would be for fully automated handling of mail-in samples or remote user-controlled experiments. The expected Q range would be 0.005–1 Å^{-1}. This beamline also features automated sample loading and utilizes AI/ML for initial data analysis and reduction. This setup makes it ideal for high-throughput, remote access, and automation-driven studies, catering to both academic and industrial users. The beamline is optimized for sample screening before in situ or operando experiments on other SANS instruments. Scientifically, RoboSANS serves applications such as collecting form factors in support for neutron spin echo experiments, metallurgical contrast checks on ex situ samples, and contrast matching for soft matter and biological samples. It is suited for handling conventionally sized samples and could potentially streamline industrial sample analysis.

Metallurgy and Geology SANS

This instrument would be designed as a high-flux, medium-resolution SANS beamline, which is ideal for handling metallurgical and geological samples. The emphasis would be the need to handle highly radioactive samples, thus requiring special shielding and remote handling capabilities along the lines of the robot being used at GP-SANS and Bio-SANS. This beamline would be very much like the current reactor SANS instruments that are classified as 40 m SANS (20 m collimation, 20 m sample-to-detector distance). It would be built to include a full multiframe detector that is proposed at GP-SANS. This capability would allow for a large dynamic *Q* range collection at one setting, which would enable time-resolved modes and kinetic studies. This beamline would be designed to incorporate a fully polarized beam when needed for study of magnetic metallurgical samples. The science emphasis for this beamline would focus on precipitate growth in reactor pressure vessel steels, the changes in microstructure in new complex high-entropy alloys, pressure effects on geological and metallurgical systems, thermal evolution in metals, advanced ceramics, and geological systems with emphasis on studying porosity and pore accessibility. It could also be modified for energy storage, filtration, and waste removal applications. To achieve these science missions, the beamline would need to have a large open sample space that would host a large selection of sample environments, including 2 kN load frame, diamond anvil cells, gas pressure cells, vacuum and air furnaces, wide-angle opening 2 T vector magnet, cryostat, and robot for rastering and highly radioactive samples.

Fundamental Physics Beamline

The demand for such an instrument will depend on the future of NCNR and their plans for a new reactor. NCNR has decades of experience in fundamental neutron physics, and that community would benefit from optimized instruments at HFIR if NCNR ceases operations. The instrument would ideally be placed at the end of a cold neutron guide, well isolated from neighboring instruments. Experiments could utilize monochromatic beams and/or neutron interferometry.

Polarized Cold Neutron Single-Crystal Diffractometer

Cold neutrons allow the use of polarizing optics. Such optics can provide very high polarization efficiency and high flux when coupled with a high-reflectivity monochromator such as PG (002). Additionally, an array of these optics can be placed after the sample, providing the ability to perform full polarization analysis over a wide range of scattering angles (e.g., the D007 instrument at ILL). This configuration can enable unique exploration of diffuse scattering, including separation of nuclear-coherent, magnetic, and nuclear-spin-incoherent contributions.

Multicrystal Reflectometer

At a continuous reactor source, the productivity and performance of a reflectometer can be boosted by using a white beam on sample and then taking reflected intensities through a set of multiple analyzer crystals and detectors to measure many reflections simultaneously. The CANDOR instrument at NCNR has pioneered this concept. This instrument can be realized with many analyzers, individually aligned to reflect a given wavelength to a particular detector. To the degree possible within geometric constraints, the detector and analyzers can also be chosen to provide spatial imaging of the scattered beam.

High-Resolution Backscattering Spectrometer

Design of reactor-based neutron backscattering spectrometers has been perfected by the instruments such as IN16B at ILL, HFBS at NCNR, and SPHERES at Heinz Maier-Leibnitz Zentrum. Thus, a high-resolution backscattering spectrometer at HFIR is envisaged to largely replicate the components inside the vacuum vessels of the existing backscattering spectrometers, utilizing a phase-space transformer, a Doppler drive-mounted silicon (111) monochromator, and a large array of silicon (111) crystal analyzers of ~2 m radius. Improvements in guide optics compared with the existing backscattering spectrometers are possible. Compared with the time-of-flight backscattering spectrometers such as BASIS, reactor-based backscattering spectrometers have better energy resolution (≤1 μeV) and provide better quality data for the temperature-dependent scans of the energy-resolved “elastic” scattering intensity because they can “condense” a band of incident neutron energies into the narrow elastic intensity line. For example, BASIS and HFBS are highly complementary, as evidenced by numerous shared publications.

Additional Cold Neutron Triple-Axis Spectrometer

MANTA will provide world-leading capabilities for cold neutron triple-axis spectroscopy. Comparison with other reactor-based neutron scattering facilities shows that most facilities have two cold triple-axis spectrometers, but HFIR only has plans for one. A second instrument provides an opportunity to optimize each for different purposes (e.g., a simpler single-analyzer detector configuration on one instrument and a multianalyzer configuration on the other). Cold triple-axis instrument concepts have evolved significantly in recent years with multianalyzer concepts such as CAMEA, MARMOT, and HODACA being tested and installed. A second spectrometer allows complementary multianalyzer approaches to be deployed.

Prompt Gamma Activation Analysis

Cold-neutron prompt gamma activation analysis is a nondestructive analytical technique for bulk multi-elemental analysis. Detection limits vary with the neutron capture cross section, but most elements are sensible within the microgram range. Applications are diverse, including archaeology, medicine, environmental science, catalysis, irradiation testing, and materials science. A combined prompt gamma activation analysis facility with neutron depth profiling would enable bulk and surface elemental analysis akin to the NPD instrument at Heinz Maier-Leibnitz Zentrum . A key strength would be in energy storage (i.e., battery) research by leveraging the high capture cross section of ^{6}Li.

Appendix: Instrument Advisory Board Report from 2018

Report of the ORNL Neutron Sciences Instrument Advisory Board
January 24 and 25, 2018

Summary

The Instrument Advisory Board (IAB) of ORNL Neutron Sciences Directorate met on January 24-25, 2018 to discuss future neutron instrumentation at ORNL over the next 10 to 15 years. ORNL currently operates two neutron sources, the First Target Station (FTS) at the SNS which provides intense pulsed neutron beams optimized for short pulses and thermal neutrons, and the High-Flux Isotope Reactor (HFIR) which provides high time-averaged brightness of both cold and thermal neutrons. Instrumentation at these sources provides excellent capabilities for a broad range of scientific applications.

Over the next dozen years or so, ORNL expects to build and commission a second target station (STS) at the SNS which will be optimized for cold neutrons and high brightness. The IAB was excited to hear about the recent progress that has been made in designing very bright parahydrogen moderators for the STS. The ability to examine a scale model of the STS target/moderator system was also illuminating. The new moderators provide fresh opportunities to optimize instrumentation across the three sources (FTS, STS and HFIR) and exploit their complementary capabilities. ORNL must also coordinate further improvements to their existing instruments with the construction of new instruments across their three sources. It is important that ORNL proceed with a holistic approach that optimizes the placement of new instruments across these sources to maximize their overall neutron scattering capabilities and scientific impact now and into the future.

This report summarizes the IAB's discussions and provides suggestions for future instrumentation at ORNL. The key assumptions of this report are:

a) the STS will be completed (or nearing completion) at the end of this time frame;
b) HFIR will operate throughout this period, except for a year-long outage to replace the Be reflector, and will continue for a significant period into the future;
c) the First Target Station (FTS) at SNS will continue operations throughout this period.

This set of assumptions is referred to as the "three source vision" for neutrons at ORNL. If any of these assumptions are not met, our advice would be altered.

Just as importantly, the final optimization will require detailed simulations of the way instruments perform at each of these three sources. This means that final decisions about the instrument suite cannot yet be made definitively. This meeting of the IAB was very timely because the board could discuss a broad range of issues and provide input during the decision-making process. Thus, the input in this report should be taken as part of the evolving optimization process: as simulations are performed our advice might indeed change. With these caveats, the following recommendations are in our priority order.

1) *The IAB recommends that ORNL add new instruments to the FTS.* The imaging station, VENUS, should have the highest priority. An imaging station would likely help ORNL better engage industry and would provide a large field of view and energy resolved capability unmatched in the US. The nation is also in need of more capacity and enhanced capabilities for neutron powder diffraction, both for traditional Rietveld refinement and for pair distribution function (PDF) analysis. Thus, the committee believes that the two additional powder diffractometers, DISCOVER and HiResPD, should also be built at FTS with high priority. The combination of these two instruments would round out the powder diffraction suite. Moreover, these instruments fit extremely well into the three source vision

providing capabilities on the first target station that would not be superseded by the performance of instruments at the STS. We realize that the construction of HiResPD requires relocating instruments and the IAB sees no disadvantages with the proposed moves. We believe that it is essential that this be done as soon as possible.

While the three-source vision appears to be well developed for the operation and development of FTS within the context of STS, the role of HFIR within this context was less clearly articulated. *The IAB believes that ORNL must deliver an impactful and sustainable plan for HFIR that exploits its high time averaged cold and thermal brightness.* ORNL should balance the entire instrument suite across all three sources as well as the capabilities at NIST. We acknowledge the complexity of optimizing such diverse opportunities across the sources, and emphasize that rational choices cannot be made without detailed simulations.

2) *The IAB recommends that ORNL update and optimize the thermal neutron instrument suite at HFIR to provide the US neutron community with internationally competitive instrumentation.* The HFIR thermal brightness will not be superseded by either FTS or STS. Thus, providing the US scientific community with state-of-the-art thermal neutron capabilities at HFIR is essential to effectively realizing the three-source vision. In light of these considerations, ORNL must develop and implement a renewal plan for the outdated thermal instrumentation at HFIR.

3) *The IAB recommends that ORNL finalize plans for upgrading the cold neutron delivery system at HFIR.* The cold source at HFIR is very bright. Unfortunately, the geometry of the HB4 tube where the cold source is located imposes severe geometrical challenges on the efficient transfer of large numbers of neutrons to the guide hall. Thus, this source is ideally suited for instruments where brightness is the primary consideration *e.g.* SANS and neutron spin echo (NSE). The IAB agrees that ORNL must take advantage of the replacement of the Be reflector as an opportunity to improve the delivery of cold neutrons. As part of this upgrade, ORNL should enhance the cold neutron instrumentation at HFIR.

   a) *The IAB recommends that ORNL develop a national roadmap for NSE.* The US scientific community lacks access to an NSE instrument capable of measuring the same range of time scales as IN15 at the ILL, placing them at a significant disadvantage. ORNL has stated that they don't currently have the expertise to build an NSE and that they will begin to gain that expertise when the FTS NSE is transferred from Jülich to ORNL two years from now. The IAB feels that this approach is too casual for an instrument that has been repeatedly identified as a high priority by the US scientific community. Providing such a capability in the US will be a major undertaking which requires substantial contributions from international experts. This should be informed by the previous workshops and the three source vision.

   b) *The IAB believes that ORNL should develop a modern guide and the primary spectrometer for a new cold triple-axis spectrometer.* The cold triple axis, CTAX, has long suffered from poor neutron transport from the cold source and urgently needs to be upgraded. We recommend that ORNL should initially use the secondary spectrometer from CTAX. The instrument should be compatible with Larmor precession methods. MANTA is consistent with the three source vision as it is unlikely that the capabilities of this instrument will be superseded by STS.

   c) *The IAB believes that the new cold guide system should not degrade the performance of the cold imaging station and should enhance it if possible.* Neutron imaging also relies largely on brightness, though field of view is also an important consideration. Alternatively, the cross-source optimization could result in this instrument being relocated to a thermal neutron beam after the Be-reflector outage.

d) *The IAB believes that ORNL should NOT build a new SANS in the HFIR cold guide hall.* While the IAB believes SANS is important, an additional SANS is not essential in the national context. Already 20% of the neutron scattering instruments in the US are SANS machines and thus this would only increment that SANS capacity slightly. Rather, ORNL should consider building two new SANS instruments at the STS one of which should be something like SWANS. The IAB believes that this is a better option than building a third SANS instrument in the cold neutron guide hall that would be moved to the STS when complete, providing only a few years of operation at HFIR. It is not clear how this would advance the three source vision and the resources that would go into moving the instrument would be better spent elsewhere.

The instruments outlined as high priority concepts for STS appear to be appropriate to the new source and have a good level of technical and scientific ambition. *The IAB encourages the continued development of these STS concepts and to further explore possibilities such as a 2nd SANS, an imaging station, a cold version of HIGGS and a WISH-style diffractometer.* Further detailed simulations of the instrument performance should be pursued to inform any movement of instruments from FTS to STS and from HFIR to STS. Though the IAB cautions that moving instruments between sources should be pursued sparingly and only where there is a substantial performance enhancement. Wolter optics promise a way to effectively focus polychromatic neutron beams. As they would work particularly well for cold neutrons, the IAB believes ORNL should be working with NASA and NIST to advance this technology for use, particularly at STS.

I. ORNL Neutron Sources 2030, source profiles and instrument suites:

a. *Do the characteristics of HFIR, FTS, and STS complement each other in a way that allows optimal placement of instruments and neutron scattering techniques?*

The three neutron sources have very different characteristics which can be used to provide distinct and complementary capabilities. Here we describe the source characteristics and make suggestions as to how these can be exploited to provide the US scientific community access to a broad range of world-class neutron capabilities.

High Flux Isotope Reactor (HFIR)

Currently HFIR has roughly equal numbers of thermal and cold instruments, with the thermal instruments distributed on three beam-ports, and the cold instruments viewing a horizontal cold source. The time-average brightness of the thermal beam tubes exceeds that of the FTS and STS moderators by more than an order of magnitude. This translates into a strong potential for high-performance instrumentation, using focusing crystal monochromators. Fulfilling this potential requires a dramatic modernization of the existing suite of thermal instruments, prioritizing quality over the number of instruments, and bringing the remaining instruments up to the state-of-the-art at other facilities. This will involve upgraded monochromators, detectors, and shielding, along with careful simulation-based optimization. The large-area beam-tubes and best-in-class time-average brightness present a potential opportunity for thermal imaging which should be studied as part of developing a holistic approach to neutron imaging at ORNL and within the US community.

The time-averaged brightness of the cold source at HFIR exceeds that of the STS moderators by about a factor of two and of the FTS coupled moderator by about an order of magnitude. HFIR thus provides opportunities for world-class cold neutron instrumentation. However, the performance of the cold instruments at HFIR is compromised by the beam extraction arrangement, in which a rather small cold source is viewed by a guide system starting at 5 m. The proposed reduction of this distance to 4 m will improve the situation, but the cold guides will still be significantly under-illuminated for many applications. In addition, the large number of guides means that each is rather small, thus hindering the performance for many applications. The highest performance can therefore be found for instruments that rely primarily on brightness, such as SANS and neutron spin-echo. To enhance the instrumentation at HFIR, potential increases in cold source brightness and further significant reduction in the moderator-guide distance should be studied. Taken together, these could dramatically increase the cold-neutron performance, particularly for instruments which require large phase space volumes such as triple-axis instruments with large double-focusing monochromators.

Finally, HFIR should exploit the comparative simplicity of monochromatic instruments for polarized-neutron applications, such as spherical polarimetry and novel precession techniques.

SNS First Target Station (FTS)

The FTS has a mature suite of instruments which are well-suited to its source characteristics. Once the STS comes online, a small number of instruments should be considered for relocation to the STS to benefit from the excellent cold neutron performance that source. The IAB recommends that when new instruments are built at the FTS over the coming years, a view is maintained of the expected STS parameters, so that the new instruments do not end up having to be relocated. It is clear, however, the FTS will remain a very attractive option and will continue to be the source of choice for many applications.

The decoupled and poisoned moderators provide pulse widths which are better-suited to high-resolution applications. That is the case both for thermal/epithermal neutrons where the water moderators provide significantly sharper pulse widths than the STS moderators, as well as for the cold moderators, where the pulse width can be up to an order of magnitude less at long wavelengths. Since very long flight paths are not available at the STS, these short pulse widths are the only means of reaching the high wavelength resolution needed for high-resolution spectroscopy and diffraction.

While the peak brightness of the FTS and STS moderators are very similar for neutron energies above about 100 meV, the higher repetition rate of the FTS provides a significant gain at these energies.

The viewed moderator surface at the FTS is typically of the order of 100 cm^2 or more. This further enhances the performance of instruments using epithermal neutrons where guide transport is less effective, allowing short instruments to let the moderator illuminate the sample directly, while still delivering a sufficient beam divergence to reach the required high flux at the sample. Similarly, an imaging instrument placed at the FTS can view the moderator directly, without using a neutron guide. This will provide a very uniform illumination of a relatively large field of view, minimizing systematic errors arising from the unavoidable beam divergence structure associated with reflective neutron optics.

<u>SNS Second Target Station (STS)</u>

The STS will be the world leader for peak cold neutron brightness, a key parameter for high wavelength resolution neutron scattering instruments. Of the three sources, it will also provide the highest peak brightness of thermal neutrons. It will therefore be the source of choice for many neutron instruments.

The increased peak brightness of the STS will be game-changing for many cold neutron applications. It will be an excellent source for reflectometry, medium-resolution spectroscopy, and high-intensity instruments that require only moderate wavelength resolution, such as SANS and spin-echo.

The high source brightness is achieved partly by reducing the viewed size of the source, which lends itself to producing small, intense beam spots. This is perfectly suited to measuring small samples, or small parts of larger, sometimes inhomogeneous sample.

The very fast measurement times enabled by the high peak brightness will allow systems to be studied which vary on the second-to-millisecond timescale.

The 15 Hz repetition period will result in a large bandwidth of neutron wavelengths reaching the sample, allowing the coverage of several orders of magnitude in length or time on a single instrument.

b. *Are there emerging techniques that should be considered for placement at one of the sources?*

Work on several new techniques was presented to the committee, including Larmor labeling, spherical neutron polarimetry, dynamical nuclear polarization and Wolter optics. Each of these efforts appears to be well-supported and making significant and steady progress and there will likely be multiple opportunities for deployment at each of the three sources in the future. The IAB encourages on-going evaluation of the integration of these techniques into user instruments depending on the success of current R&D efforts. In the past, it has taken some time for new neutron methods to be adopted by the broader user community and we would expect the same phenomenon to manifest with these new techniques. Success will likely be tied to the demonstration of significant scientific advances that are enabled by the new methods.

Wolter optics

The continuous development of advanced neutron optics has been one of the primary avenues of creating ever more capable neutron instrumentation. Wolter optics, a reflective lens, are the most promising new technology that can continue this trend into the future. These lenses, which can focus a polychromatic beam, are made of Ni and work best for cold neutrons possibly providing gains of more than an order of magnitude. These are far beyond the early development stage as NASA has launched these optics into space as part of the Chandra x-ray telescope. While these lenses were deposited on glass substrates, they are now making these optics from free-standing films. In collaboration with other facilities and the MIT effort, the IAB believes that ORNL should consider how to contribute to advancing this technology.

Detectors

With the ^{3}He crisis in the mid-2000s, many neutron facilities accelerated their detector development programs to replace ^{3}He detectors. To better coordinate these efforts, a large collaboration was initiated among major neutron facilities in 2010. ISIS, SNS, J-PARC and PSI worked to further develop scintillation detectors, while the ILL, ESS and other European facilities participated in B-coated detector development and in refurbishing BF_3 detector technology. Even before this, ORNL developed a scintillation detector system that was deployed on POWGEN, VULCAN *etc.* Unfortunately, there have been some issues with these detectors and VULCAN is replacing theirs with ^{3}He detectors and POWGEN is moving to newly developed scintillation technology. We trust these new detectors will perform well. Note however, that scintillation detector systems at ISIS and J-PARC have been working well and NIST has just developed new technology for the fabrication of scintillation detectors that enhances their performance. The IAB believes it is important for ORNL to continue to develop scintillation detector systems and to exchange technical information with other neutron facilities.

Computing

Computing is becoming increasingly important for handling and analyzing neutron scattering. For example, DFT calculations are routinely done in conjunction with neutron vibrational spectroscopy. Moreover, the volume of data generated by certain ORNL instruments is too large to be treated by researchers using the computing infrastructure at their home institution. ORNL is a center for high performance computing. Therefore, the IAB believes that ORNL should work to further develop synergies between high performance computing and neutron measurements.

Moderator and reflector

The detailed cross section of H-molecules only became available in late 1990's. This was too late for the FTS design to benefit from the use of para-hydrogen in the moderator design. J-PARC has since shown the performance advantage of para-hydrogen with a pre-moderator, and now all new H_2 moderators are using this technique to enhance performance. The ESS has made additional improvements, developing a low-dimensional moderator system. STS is taking full advantage of this knowledge, experience and technology. While the FTS is not optimized for para-hydrogen moderators, it is worth studying the neutronics performance gain, and perhaps include a para-hydrogen converter in the H_2 cryogenic circuit when there is a major replacement of the target and moderator system.

Quite recently, the ESS has discovered that the performance of the Be reflector is very sensitive to the texture and quality of the material. While this is an ongoing development, it may provide an avenue to improve the Be reflector at HFIR.

Pulse shaping and multiplicity

Repetition Rate Multiplicity (RRM) was first demonstrated in the 1990's. RRM has now become a normal operational mode of several regularly operating instruments. Since this technique is indispensable for a long pulse neutron source, most of ESS instruments are designed with RRM in mind. Since FTS operates at 60 Hz, the use of RRM there has been limited. However, STS will produce a broad peak with a much lower repetition of 15 Hz. Therefore, the use of RRM can benefit inelastic scattering instruments at the STS. A chopper can be used to sharpen the peaks produced by the STS moderators making an instrument high resolution. The IAB believes that instrument designs for the STS and the decisions of which instruments to move from FTS to STS should also take these considerations into account.

Nano diamond reflector for beam extraction from moderator

There is a program coordinated by IAEA that aims to drastically improve available neutron fluxes. One idea being explored is beam extraction using nano-diamonds. This material is very durable even in a high radiation fields and can be placed at a short distance to the source. Recent results are quite promising for cold neutrons. Although this technique is under development and a robust fabrication method must still be realized, it is worth studying the performance of this technique for the STS and HFIR.

c) *Have we maintained sufficient flexibility in our plans to allow for future innovation in instruments and methods?*

In the context of the three source vision it is not at all clear that the heavy focus on squeezing every single neutron out of the HFIR cold guide hall, even the less than optimal CG4, is the best use of limited resources. Firstly, if further simulations confirm that the long term strength of HFIR is its thermal capabilities, it would seem that limited resources would be better spent focusing on modernizing, prioritizing and innovating the thermal instrumentation suite as recommended in the "2017 Review of the Instrument Suite for Inelastic Scattering" report. Such an optimization should include re-prioritization of instruments, considering removal of instruments that will do significantly better at the FTS or STS, adding new high impact instruments such as a thermal imaging station for example, and fully updating/upgrading the world class thermal triple axis (including the not yet approved upgrades to some of the backends).

The cold neutron guide hall at HFIR is at capacity. The Be-reflector replacement will provide an opportunity to reoptimize the instrument suite. ORNL should take this opportunity to develop a modern cold triple axis – an instrument which will not be superseded by the STS. ORNL should also carefully consider imaging in light of the three source vision with the aim of providing the best instrumentation for the US for this emerging technique. It is also essential that a ORNL develop a plan for NSE that results in an instrument competitive with IN15 at ORNL. Further, a 3rd SANS will only increase the US capacity by about 10-15% and the plan to move it to STS later along with the other two SANS instruments currently at HFIR, fails to address the role of the HFIR cold guide hall in the three source vision and leaves a big gap in its instrument suite.

Making a beamline available at SNS as a test station is an important component for maintaining flexibility. This test station might have a modular design to make reconfiguration easy. A test station will be especially helpful for aiding in the design of instrument concepts that have yet to be built anywhere else, developing proof of principle concepts and technologies for STS. The ORNL team has proposed such an instrument before (INVENT) although it was not discussed and not considered a high priority.

Building new instrumentation in a modular fashion maintains maximum flexibility. However, the IAB feels that a modular approach for easily moving beamlines could be counterproductive as any such move could severely inconvenience the scientific community.

A critical point, and one regularly mentioned but often ignored in practice, is the fact that the productivity of an instrument depends on much more than its performance. The IAB strongly encourages ORNL to take a holistic approach to instrument design rather than simply provide "flexibility" for everything else. This means thinking about sample environment and software development needs (not only data acquisition but reduction and analysis) as an integral part of the instrument planning phase. Maximum productivity of any instrument will only be met when considering all these aspects of an experiment. For example, if a new instrument collects data at a much higher rate than current instruments, sample environments must not become the rate limiting step. If necessary, new technology in sample environment must be realized simultaneously with instrument implementation. Space must also be well thought out to allow for the flexibility of different sample environments required by users. Also, if adequate, user-friendly software is not developed to handle the large amount of data generated by a new instrument, then productivity will not improve. Therefore, it should be a top priority in the development of any new instrument to make a comprehensive plan that includes every aspect of importance to the user.

Finally, it should be emphasized that there is a critical need to maintain space in the budget to allow for integration of future innovations into the proposed new instruments. In this context, the lack of nearly $6 million to complete the proposed instrument buildout with the plan to get partners to make up the slack is a bit worrisome. It is not clear that such partners can be found given the constraints of the facility and an open access beamline. It would be prudent for ORNL to seek ways of developing and funding these instruments completely rather than piecemeal. While some of these funding avenues could involve innovative ways of engaging industry to have a role in instrument development, the facility should think more broadly about alternative funding streams as well as a contingency plan should such funding not be forthcoming.

II. **Priorities for improving existing instruments and building new instruments at FTS and HFIR**

a. *Do the current ORNL instrument suites represent a balanced portfolio of capabilities that is expected from a major center for neutron scattering?*
b. *Are there gaps in capabilities or capacities we have identified that should be addressed with high urgency? Are the priorities identified for near term (0-5 years) investment appropriate?*

Imaging

Neutron imaging is a powerful technique for the 3D visualization of materials that range from fundamental new systems through to device components; complementary to other techniques, neutron imaging offers unique insights into the materials world and, as such, it is essential that neutron facilities provide this capability. ORNL, with its existing facilities, HFIR and FTS, and the future opportunities afforded by a STS, has the potential to provide a world-leading suite of neutron imaging instrumentation. Currently, CG-1D, the cold neutron imaging instrument at HFIR, is the only imaging facility at ORNL. With limited resources, CG-1D has produced a significant amount of valuable research. The proposal to construct VENUS, a platform for studying materials and engineering components on the FTS, is an important and essential development in establishing ORNL as a world-leading neutron-imaging institution. VENUS should be operational by the time of the HFIR outage so that ORNL maintains a neutron imaging capability throughout this period. Finally, ORNL must develop a plan for imaging taking into account the three source vision. This plan should consider the potential of imaging instrumentation using both thermal and cold neutrons at HFIR and at the STS in addition to VENUS and the cold neutron imaging station at HFIR.

Diffraction

Single crystal diffraction covers a very broad range of science from the detailed diffuse scattering of fundamental condensed matter systems through to biological macromolecular crystallography. There is an existing extensive portfolio of single crystal instruments at HFIR and SNS-FTS. Careful consideration, over the next five years, of future opportunities should be undertaken with a view to rationalizing single crystal instrumentation on HFIR, FTS and a future STS to ensure the optimal coverage of the future scientific challenges in neutron single-crystal diffraction.

Powder diffraction is a key technique for the characterization of both fundamental and applied materials systems. The current powder diffraction instrument suite at ORNL produces high quality science but is outperformed in many areas by the instrumentation at ISIS and J-PARC. The near-term construction of DISCOVER and HighResPD is essential to establish ORNL as a world leader in neutron powder diffraction (NPD). DISCOVER builds on the existing excellence at ORNL in NPD and, in particular, PDF analysis, and will result in world-leading capabilities in combined NPD and PDF. HighResPD will provide high flux and very high resolution that is comparable with synchrotron X-ray powder diffractometers. HighResPD is necessary for the complementary analysis of X-ray and neutron powder diffraction measurements of structural complexity ranging from subtle structural phase transitions in fundamental materials to microstructural imperfections associated with real world issues such as catalysis, battery cycling and materials degradation. The recent decision to move HighResPD from an STS instrument concept to a shorter-term project for FTS makes sense for several reasons. First, it will bring this much needed capability online sooner. Second, HighResPD can be implemented at FTS with little performance impact and is consistent with the three source vision. It also allows the STS design to be fully optimized for cold, low- to medium-resolution applications, without compromise. In preparation for a future STS, it is important to consider, in the near future, the opportunities afforded by a medium resolution, cold-neutron powder diffraction (WISH-type) and a medium resolution combined high Q and small-angle total scattering instruments (SWANS).

Spectroscopy

FTS and HFIR have extensive capabilities in neutron spectroscopy for quantum materials, chemistry, and catalysis. The clear capability gap in this suite is cold-neutron triple-axis spectroscopy, which most directly affects quantum materials research. While the CTAX instrument fits this profile, the low flux and lack of polarized beam capability limit its scientific impact. A competitive cold triple-axis spectrometer is needed at HFIR to complement the highly productive CNCS instrument at the FTS. The MANTA instrument concept is currently being developed and has strong community support. ORNL must strongly pursue simulations of MANTA to confirm its performance as world-class instrument.

Investment in MANTA, and the cold source in general, must be balanced with the urgent need to modernize thermal triple-axis capabilities. These instruments have not been updated in decades. Newer concepts in thermal triple-axis spectrometers (such as a multianalyzer backend) have been employed at other facilities with great success. Here it seems that the opportunity and indeed the necessity of reoptimizing the cold guide hall during the outage for the Be reflector conflict with the long-term three-source vision which places emphasis on HFIR's capabilities as a premier thermal neutron source. ORNL should think carefully about this tension and come up with a plan that also ensures the long-term sustainability of the HFIR thermal instrument suite. As an example of a particular trade-off, the IAB notes that most of the improvement on MANTA will come from the improved guide system. We therefore believe that ORNL should operate MANTA with the current CTAX secondary spectrometer.

The HIGGS inverse geometry spectrometer was proposed as new instrument concepts for FTS. As HIGGS covers similar science as the thermal direct geometry spectrometers, there is not an urgent need. However, the concept should be explored as it promises to deliver much higher counting rate, albeit with reduced flexibility and the potential for much higher background. This is a concept that can be more straightforwardly employed with cold neutrons and should be explored for STS.

BeFAST is another proposed inverse geometry spectrometer that would be a low-resolution version of VISION. It would extend capabilities for chemical spectroscopy, but is not an urgent short-term need.

Neutron Spin Echo

Traditional energy-resolving neutron spin echo (NSE) is critical for soft matter researchers, as it provides unique sensitivity to very slow motions inaccessible by other techniques (neutron or otherwise). Unfortunately, the NSE situation in the US is far from satisfactory. Currently the US scientific community lacks access to an instrument capable of measuring the same time-range as IN15 at the ILL placing them at a significant disadvantage. The single NSE instrument at ORNL is not globally competitive and there is little the SNS can do about this until they are able to take full responsibility for the instrument in 2020. Per the 2017 inelastic suite review, BL-15 at SNS is limited to a maximum Fourier time of 150 ns. The only other NSE in North America (at NIST) can measure out to 300 ns, while IN15 at ILL regularly measures out to 600 ns. In principle, a new NSE competitive with IN15 could be constructed at an end guide position viewing the HFIR cold source although it is possible that the STS would be the best long-term source. ORNL proposed to attempt to double the maximum Fourier time of the existing NSE through the installation of new compensation coils sometime after 2020. The IAB believes that this approach is inadequate, rather it is essential that ORNL produce a long-term approach to developing a truly forefront NSE instrument in the US. The IAB understands that this will take a major effort requiring significant contributions from international experts. A final plan needs to be based on a detailed technical evaluation that includes a complete understanding of the reasons for the disappointing performance of the NSE at the FTS. Given significant current need and the long lead time for developing such an instrument, it is imperative that ORNL begin the process immediately.

SANS

The ORNL SANS suite features 3 SANS instruments plus a USANS instrument. All are oversubscribed, and the proposed addition of a new SANS in the HFIR cold guide hall would certainly be well utilized by the US scientific community. However, there are already 9 SANS instruments, including 7 pinhole machines in the US providing a wide range of capabilities. Therefore, the additional capacity provided by an 8th pinhole SANS instrument is not very compelling. In addition, the idea to build a new SANS in the HFIR cold guide hall, and then move it to the second target station (STS) would cost significant resources and disrupt the SANS user program. Given that there are critical gaps that the facility should address, and that SANS instruments are expected to perform very well at STS, it is sensible to avoid moving instruments to the extent possible, and plan for one and probably two SANS specifically designed for placement in the STS. The IAB believes that the planned move of USANS to HFIR should be pursued. It will improve performance while freeing up needed real estate at FTS.

Reflectometry

ORNL currently operates two world-class reflectometers at FTS. Capabilities exist for liquid samples, vertical geometry, polarization, and polarization analysis. A third reflectometer for the HFIR cold guide hall was proposed as a low priority. We agree that this is a low priority and instead recommend focusing on reflectometry at the STS, where truly game-changing instruments can be constructed.

c. Are we effectively identifying and realizing new opportunities in neutron sciences that could be optimally addressed at FTS or HFIR?

One clear gap in US capabilities which has been pointed out by several panels and committees, including the "2017 Review of the Instrument Suite for SANS/Reflectometry…" is the low q, long time scale dynamics that an IN15 class spin echo machine would provide. This is particularly important for the soft matter community. Combining structure with dynamics is emerging as the next challenge akin to the multiscale challenge of the past decade that SNS and HFIR have been working to address in all their new instrumentation. There is currently no such capability in the US and the HFIR cold source is currently the only place such an instrument could be built, thus presenting a unique opportunity. While the IAB appreciates the risks may be quite high given the expertise of the lab and complexity of the instrument, we strongly recommend that this option be considered more carefully and that a plan be developed immediately that will result in an NSE instrument that is competitive with IN15.

The closure of two major neutron sources in North America (the Lujan Center at LANSCE in New Mexico and Chalk River National Laboratory in Canada) has resulted in a crisis for the scattering community. The Lujan Center, for example, was a mecca for nPDF (neutron PDF) analysis of disordered materials. ORNL is proposing to build DISCOVER - which will fill a need for nPDF in North America. Much of the Lujan talent has already relocated to ORNL and there is an opportunity for ORNL taking a real leadership role in this area which they should fully embrace. Similarly, Chalk River was a center for applied neutron diffraction through the ANDI program (Applied Neutron Diffraction for Industry). This is another opportunity to build upon this expertise with applied neutron diffraction on instruments such as VENUS (building on the success of instruments such as VULCAN).

d. Are we missing critical areas for further scientific and technical innovation?

Studies of heterogeneous materials, especially soft matter and glasses, have begun to show that imaging correlations in real-space and time through the correlation function G(r,t) can sometimes provide scientific insights not available by looking at S(Q,E). This method often requires that data from various spectrometers, each covering different Q and E ranges with different resolutions, to be combined and Fourier transformed. The procedure requires careful statistical treatment using, for example, maximum entropy methods and has not yet been widely adopted. Opportunities may also be available to measure G(r,t) directly using Larmor labeling techniques over suitable ranges of r and t. These areas may be an opportunity for ORNL to take a lead in view of the wide dynamic ranges of its spectrometers, their institutional excellence in computing and their emerging expertise in Larmor labeling methods.

The need to access a wide range of parameter space is becoming increasingly important, as the systems under study become more complex and more in-situ and in-operando measurements are performed. This will benefit from the construction of instrumentation where neutron methods are combined, such as: spectrometers with diffraction capabilities which allows following dynamics and excitations through a well characterized phase diagram; diffraction instruments that probe a wider range in Q-space realized as a SANS instrument designed with a medium angle detector or a diffractometer with a SANS detector (SWAN proposal); and/or wide energy coverage in reciprocal space via combining direct and indirect spectroscopy methods.

The high brightness of SNS and HFIR sources provide opportunities to observe phenomena in a real time (kinetics) and to perform faster measurements (high-throughput), but these experiments must be enabled by appropriate resources. To this end, automation should be seriously explored for sample loading and changing, as well as remote handling and software for data reduction and analysis. Similarly, in-situ and in-operando measurements are in high demand (e.g. catalysis or conventional chemical reactions, recent experiments on VULCAN on an operating engine, polymer processing), enable new and exciting science and discoveries, and attract interest from industrial stakeholders. Careful consideration of the implications on the instrument scientist and sample environment teams in terms of design and operation of new equipment, as well as time and staff effort is imperative. Furthermore, an engagement with the existing user community and outreach into new ones are key to identify demands alongside a strategic deployment.

An easily reconfigurable test beam port has an important role for various development purposes, including detectors, optical components, methods development *etc*. Beam ports that lack sufficient space for a full-scale neutron instrument would be a reasonable place for a test station such as INVENT. Although there is a test port at HFIR, pulsed neutrons provide unique capabilities that make such a port essential, particularly considering the need to develop ideas for the STS. We thus encourage SNS to make such a port available.

Consideration should be made of the use of the epithermal neutron spectrum available at SNS for testing single event effects and more generally for neutron irradiation. A beamline dedicated to this, similar to the ChipIr instrument at ISIS TS2 would provide a unique capability to the US community.

Since SNS is funded by the Basic Energy Sciences division of DOE, industrial use of the facility has not been aggressively pursued. However, neutrons are becoming increasingly important to industry. J-PARC is a good example, where more than 30% of experimental proposals come directly from companies. There are also new efforts in Europe, to encourage industrial use of neutron and photon facilities. It is worth looking at a recent Focus feature in the October 2017 issue of Physics World magazine, on "How industry exploits neutrons". Often industry is unaware of how neutrons can help their companies and thus, suitable outreach efforts are required to stimulate them to use neutrons.

Thanks
The IAB thanks ORNL for the hospitality and their openness in presenting their ideas. We also appreciate that ample time was provided for discussion in executive session. It certainly made our job easier.

APPENDIX A - Charge

Instrument Advisory Board
January 24-25, 2018

Background
Over the past three years we began 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. We established a mechanism (the Science Productivity Process) and a rolling budget to enable these goals. The Science Productivity Process has already provided new capabilities. We have now completed the first series of planned triennial reviews of the instrument suites at SNS and HFIR.

We now look to the future and what the next steps will be for further improvements to existing instruments and for the coordinated construction of new instruments. Over the next 5-10 years, there are opportunities to build new instruments at the remaining 5 open beam ports at the SNS First Target Station (FTS), to reposition instruments and to build new instruments at HFIR, and to design new instruments at a future possible SNS Second Target Station (STS). It is important that we proceed with a holistic approach that optimizes the placement of new instruments across the 3 sources to maximize our overall neutron scattering capabilities and scientific impact.

Charge Questions
We seek the Instrument Advisory Board's feedback and guidance in the following areas:

I. **ORNL Neutron Sources 2030, source profiles and instrument suites:**
   a. Do the characteristics of HFIR, FTS, and STS complement each other in a way that allows optimal placement of instruments and neutron scattering techniques?
   b. Are there emerging techniques that should be considered for placement at one of the sources?
   c. Have we maintained sufficient flexibility in our plans to allow for future innovation in instruments and methods?

II. **Priorities for improving existing instruments and building new instruments at FTS and HFIR**:
   a. Do the current ORNL instrument suites represent a balanced portfolio of capabilities that is expected from a major center for neutron scattering?
   b. Are there gaps in capabilities or capacities we have identified that should be addressed with high urgency? Are the priorities identified for near term (0-5 years) investment appropriate?
   c. Are we effectively identifying and realizing new opportunities in neutron sciences that could be optimally addressed at FTS or HFIR?
   d. Are we missing critical areas for further scientific and technical innovation?

APPENDIX B - Agenda

Instrument Advisory Board

January 24-25, 2018

Oak Ridge National Laboratory
Spallation Neutron Source, Building 8600, C-156

Event Contact: Talia Holder, 865-576-1014 (office); 865-680-1955 (cell); holdertm@ornl.gov
Organizer: Ken Herwig, 865-576-5095(office); **herwigkw@ornl.gov**

Time	Event/Activity	Lead
8:00am – 8:30am	Closed Executive Session	P. Langan M. Buchanan
8:30am – 9:00am	Directorate Overview	P. Langan
9:00am – 9:30am	Implementing the ORNL 3-Source Strategy	K. Herwig
9:30am – 10:10am	Large Scale Structures Suite	M. Fitzsimmons
10:10am – 10:30am	Coffee Break	
10:30am – 11:10am	Diffraction Suite	M. Tucker
11:10am – 11:50am	Spectroscopy Suite	M. Lumsden
11:50am – 12:45pm	Working Lunch: Dynamic Nuclear Polarization Wollaston Prisms Sphercial Polarimetry	J. Pierce F. Li C. Jiang
12:45pm – 1:25pm	Materials Engineering Suite	A. Payzant
1:25pm – 2:00pm	Neutron Scattering Division Priorities	R. Ibberson

Time	Event/Activity	Lead
2:00pm – 3:00pm	Board Discussions and follow-on questions	D. Neumann, Chair
3:00pm – 3:15pm	Coffee Break	
3:15pm – 5:30pm	Board Deliberations	D. Neumann, chair
6:00pm	Working Dinner: Title TBD	J. Galambos
	January 25, 2018	
8:30am – 9:00am	Board discussion and follow-on questions	
9:00am – 12:00pm	Board deliberations and preparation for close-out	D. Neumann, chair
12:00pm – 12:45pm	Working Lunch: High Pressure at ORNL Detector Development	TBD Rick Riedel
12:45pm – 1:00pm	Close out and Recommendations	
1:00pm – 2:30pm	Optional tours of HFIR and SNS	

APPENDIX C – IAB members

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