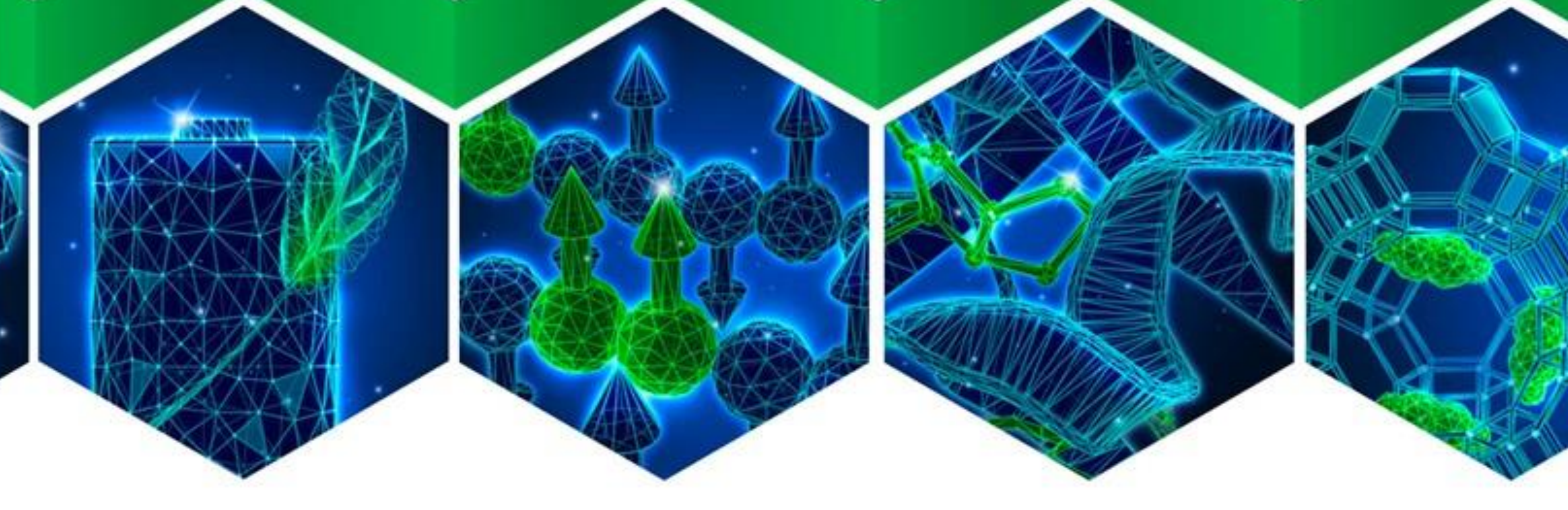
Neutron Sciences
10-Year Strategic Plan

2023 Update



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10-Year Strategic Plan
for
Neutron Sciences

2023 Update

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EXECUTIVE SUMMARY

The Neutron Sciences Directorate (NScD) at the US Department of Energy's (DOE's) 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 DOE Office of Science. NScD is committed to enabling the most impactful and widest possible range of research to be carried out by the scientific community by providing a powerful array of neutron capabilities for our users.

This *10-Year Strategic Plan for Neutron Sciences* articulates a vision for a future in which major societal challenges, such as delivering the clean energy transition and ensuring environmental sustainability, are addressed by advances in materials science and in which the unique strengths of neutron scattering play an essential role in enabling them, as provided by ORNL's neutron sciences facilities. In the context of recent scientific achievements, we provide examples of desired outcomes of use-inspired science of national importance. These examples highlight ambitious but achievable goals that illustrate the challenges and needs within five strategic science areas: quantum materials, soft matter, materials and engineering, chemistry, and biosciences.

This strategic plan then articulates the technical capabilities and developments that are needed to enable these science outcomes. Our technical effort directly supports our goals as illustrated by the highlighted science examples, with each of these technical developments and investments motivated by the strategic science areas that we seek to impact.

The development of our neutron sources is guided by the three-source strategy, a means to implement our vision to optimally provide neutron scattering capabilities at three complementary and world-leading facilities. This strategy includes upgrades to our sources: the SNS Proton Power Upgrade, the SNS Second Target Station (STS), and the HFIR Beryllium Reflector and Pressure Vessel replacements. Fundamental to this strategy is to place each neutron instrument at the source that maximizes its performance and to maintain investment in the sources and instrument suites to provide US researchers with continued access to world-class neutron scattering capabilities. We describe our plans for new instruments and instrument upgrades at SNS and HFIR; STS instruments, software, sample environments, and complementary techniques; and instrument technology developments; and provide a tentative timeline for the implementation of the planned capabilities and technical developments.

Scientific excellence requires operational excellence, which includes good workforce development; improvements to diversity and inclusion; a strong user program; an effective communication strategy; and world-class asset management. These facets are all underpinned by a robust culture for protecting the environment, safety, health, and quality, which are all essential to operate the facilities and to run a world-class neutron scattering program that meets the science challenges of the future and the nation's needs.

At the end of this document, we describe the important non-neutron-scattering missions of SNS and HFIR and outline a vision for enhancing the activities in the strategically important areas of isotope production, fundamental physics, and accelerator research. The combination of the neutron scattering and non-neutron scattering missions makes our facilities truly essential to the mission of the DOE Office of Science and to the nation.

The approach outlined in this plan will ensure that our neutron program is ready to meet the science challenges and national needs of the future and that the United States maintains world leadership in neutron sciences. This plan is a living document that will be updated periodically, considering community input as our strategy is implemented and adjusted as technological and scientific discoveries are made and science priorities evolve.

1 INTRODUCTION

Leadership in materials science provides the basis for a knowledge-based economy that can respond to the grand challenges that humanity faces today and in the future. A diverse materials science tool kit is needed both to address the diversity of materials science problems and to ensure responsiveness to evolving societal needs. Because neutrons have unique properties that make them a powerful probe of materials, neutron scattering is a key technique in this tool kit for advancing the science and technology of materials important in chemistry, physics, engineering, and biology. They have no charge, and, unlike electromagnetic radiation or electrons, they interact with atoms mainly via short-range nuclear interactions. For this reason, they are weakly interacting in most materials, and thus they penetrate matter far better than charged particles or x-rays. Also, unlike other common probes, neutrons can be produced to simultaneously have wavelengths and energies that are in the ideal range for the study of the structure and dynamics of soft and hard materials. The neutron cross sections are amenable to calculations that can be quantitatively compared with experiments. Because of the high-penetrating power of neutrons, neutron scattering techniques are powerful for in situ/operando and multimodal characterization of materials under a variety of conditions and processes. Neutrons interact with atoms mainly via short-range nuclear interactions, and their cross sections vary widely among elements regardless of their atomic numbers, even among isotopes of the same elements. Thus, isotopic labeling and solvent contrast variation can be used to highlight specific components of a structure with minimal perturbation of the sample properties. Finally, neutrons have a small magnetic moment that couples to the electronic spins in magnetic materials, making them ideally suited to study magnetic structures and excitations. The uniqueness of the neutron as a probe of matter and energy makes it an essential tool for the discovery and delivery of knowledge that is complementary to other probes such as photons and electrons.

The Neutron Sciences Directorate (NScD; Appendix A contains a complete list of abbreviations used in this document) at the US Department of Energy's (DOE's) 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 DOE Office of Science (SC). This *10-Year Strategic Plan for Neutron Sciences* aims to ensure that our neutron scattering program is well positioned to continue to serve the science community and to meet the science challenges and national needs of the future. The term of this strategic plan is 10 years, which is a period that will see the completion of two major neutron facility upgrades—the SNS Proton Power Upgrade (PPU) and the HFIR Beryllium Reflector Replacement (HBRR)—as well as significant progress toward both completion of the SNS Second Target Station (STS) and planning of the replacement of the HFIR pressure vessel. These plans are guided by a vision for optimum technical complementarity between HFIR and the SNS First and Second Target stations, as articulated in the three-source strategy [1], providing the platform to adapt to changing science needs and ensure US leadership in neutron sciences for decades to come.

Our goal is to provide a science-based strategic plan that identifies desired influential scientific outcomes of national importance and the technical capabilities and developments that are needed to enable them. This document comprises three main sections.

Section 2 is arranged around five *strategic science areas* in which neutrons can play a significant role and that directly address Priority Research Directions or Priority Research Opportunities identified in the DOE SC Basic Energy Sciences (BES) Basic Research Needs workshop/roundtable reports [2]. The strategic science areas are quantum materials, soft matter and polymers, materials and engineering, chemistry and environmental science, and biological materials and systems.

Each of these strategic science areas addresses one or more of the grand challenges identified in *Directing Matter and Energy: Five Challenges for Science and the Imagination* [3] while leveraging one or more of the transformative opportunities outlined in *Challenges at the Frontiers of Matter and Energy:*

Transformative Opportunities for Discovery Science [4] and addressing important national priorities within areas such as advanced and sustainable energy, quantum information science, and transformative manufacturing. The areas have been chosen so as to touch upon all five of the Critical Areas of Basic Energy Research identified by a recent BES Advisory Committee (BESAC) subcommittee report on International Competitiveness [5], and are consistent with the recommendations of the National Academy of Sciences (NAS) in the *Frontiers of Materials Research: A Decadal Survey* (2019) [6]. Selecting these strategic science areas involved soliciting and incorporating input from the user community. These areas will likely be updated as science priorities evolve and new DOE BES, NAS, and other national reports appear, together with user community input.

Within each strategic science area, we have developed a few examples that highlight ambitious but achievable outcomes that illustrate the challenges and needs of each strategic science area.

Section 3 describes the planned technical capabilities and developments that are needed to enable these scientific outcomes, including neutron sources: 10 year outlook and beyond; instrument suites at HFIR and SNS; instrument control, data acquisition, reduction, and analysis; sample environments, sample preparation, and complementary techniques; and instrument technology developments. Section 3 outlines the technical improvements that are needed to progress within the strategic science areas by linking them to the successful achievement of the highlighted science examples. These links provide the important direct connection between the technical developments and investments that are planned and the strategic science areas that we seek to impact. At the end of Section 3, a timeline for the implementation of the planned capabilities and technical developments is provided. This timeline is tentative and will be updated periodically. A list of all instruments and their locations is provided in Appendix B.

NScD's neutron facilities also provide significant and complementary opportunities for science and societal impact outside the neutron scattering mission, including radioisotope production, fundamental physics, and accelerator physics. These programs, which are described in Section 4, are inherently associated with large facilities. A high-level overview and forward-looking strategy are provided for leveraging these important investments.

Progress in materials science underpins the technologies upon which US prosperity and national competitiveness depend. NScD's strategic plan highlights how neutron science at HFIR and SNS will continue to play an integral role in that landscape.

We would like to thank the many people from the SNS and HFIR User Group, the Neutron Advisory Board, and ORNL staff who provided valuable input to the preparation of this strategic plan.

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2 STRATEGIC SCIENCE AREAS

The technologies and materials of tomorrow will depend on understanding and manipulating how atoms and molecules combine to create complex architectures that have new behaviors and functionalities. Neutrons have important properties that make them essential to this step into new levels of complexity. ORNL is committed to enabling influential and transformational research on novel materials and technologies performed by the scientific community by providing a powerful array of neutron capabilities for NScD's users. This science-based strategic plan aims to ensure that NScD's neutron scattering program is well positioned to continue to serve the science community and to meet the science challenges and national needs of the future. This *10-Year Strategic Plan for Neutron Sciences* aims to establish a direct link between the planned technical developments and investments and the strategic science areas that we seek to impact. To this end, NScD's priorities are organized into five strategic science areas in which neutrons can play a unique and significant role and that represent the user community's interests:

- Quantum materials
- Soft matter and polymers
- Materials and engineering
- Chemistry and environmental science
- Biological materials and systems

For each of these strategic science areas, a highlight of recent research at NScD's neutron facilities illustrates the unique role of neutrons in making important and transformational contributions to each of these fields. Looking into the future, selected representative examples of desired outcomes of use-inspired research opportunities address areas of special importance for the nation. These examples highlight the contributions of neutrons to solve today's most urgent technological challenges in delivering the clean energy transition and ensuring environmental sustainability, as well as national priorities such as quantum information and transformative manufacturing These examples are intended as illustrations and should not be interpreted as limiting the opportunities for research at NScD's facilities.

Special effort has been made to ensure that these examples directly address priority research directions or priority research opportunities identified in the DOE BES Basic Research Needs workshops/roundtable reports [1] as well as their grand challenges [2] and transformative opportunities [3]. These examples are also consistent with the recommendations of the NAS's *Frontiers of Materials Research: A Decadal Survey* (2019) [4]. These examples are ambitious but achievable within a 10 year horizon and are meant to illustrate areas in which ORNL neutron scattering resources are needed to play an essential role.

2.1 Quantum Materials

The physics of quantum materials cannot be explained solely by semiclassical descriptions. At the atomic scale, the laws of quantum mechanics govern the behaviors of spin, charge, and angular momentum degrees of freedom. Superconductors, magnetic materials both with and without long-range order, and topological insulators are all examples of materials for which the many-body physics of electrons yield materials that exhibit quantum behavior. Because of the unique properties of neutrons to probe magnetic materials, neutron scattering is an essential tool for the study of quantum materials, not only to provide a way to test theories of correlated electron behavior but also to provide knowledge to enable new technologies.

For example, topological superconductors are of interest because of potential applications in quantum computing. The universal origin of superconductivity is the formation of bound (Cooper) pairs of electrons that move through the lattice without resistance below the superconducting transition temperature T_c. Typically, the electrons in a Cooper pair form antiparallel spin singlets with total spin S = 0, however it is also possible to form parallel spin-triplet Cooper pairs with S = 1 with an odd parity wavefunction. Search for such spin-triplet superconductors has gained interest recently because such materials may be able to host topological states and Majorana fermions of relevance for fault-tolerant quantum computation. The most promising candidate for this type of superconductivity is UTe_2, which has $T_c \approx 1.6$ K and a proposed chiral spin-triplet topological superconducting state near a ferromagnetic (FM) instability. Although ferromagnetic (FM) fluctuations may play a critical role in mediating the spin-triplet electron pairing, recent measurements at the SNS CNCS (BL-5) instrument (Figure 2.1-1a) have revealed that the magnetic excitation spectrum of UTe_2 is dominated by low-energy incommensurate antiferromagnetic (AF) spin fluctuations [5]. This experimental work is complemented by density functional theory (DFT) plus dynamical mean field theory, which explains the observed incommensurate fluctuations in terms of the electronic structure. Furthermore, the appearance of superconductivity in this compound is coupled with a sharp "resonance" mode at a wavevector characteristic of AF order (Figure 2.1-1b–c) [6]. These discoveries, made possible by the unique properties of neutrons, suggest that AF spin fluctuations may drive spin-triplet superconductivity with the potential to host technologically promising topological states.

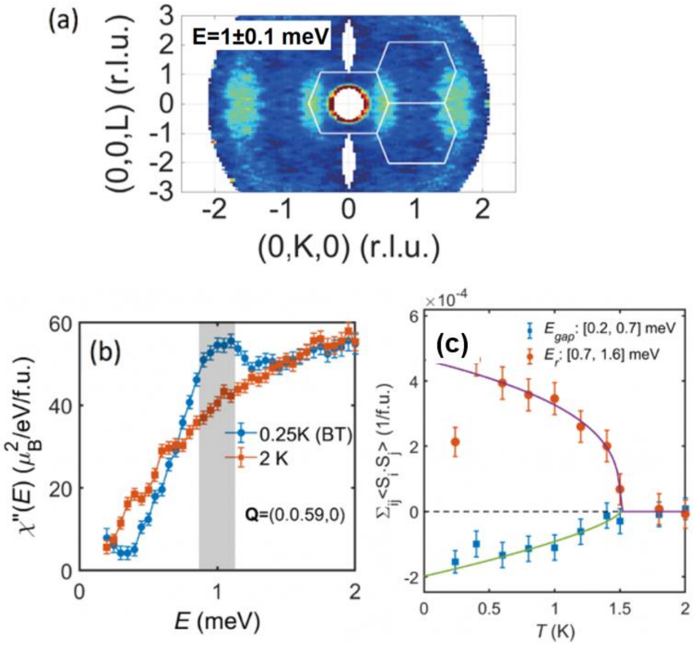

Figure 2.1-1. Antiferromagnetic fluctuations in the spin-triplet superconductor UTe_2. (a) Intensity map in the (0,K,L) plane at an energy transfer of 1 meV showing that strong magnetic fluctuations occur in UTe_2 at incommensurate wavevectors centered at $G \pm (0, 0.57, 0)$ where G is a reciprocal lattice point. Reprinted from Duan et al. 2020 [5] with permission from the authors. (b) Energy dependence of the imaginary part of the dynamical susceptibility ($\chi''(E)$) centered at the wavevector $Q = (0, 0.59, 0)$ for temperatures of 0.25 K and 2 K (below and above T_c). (c) $\chi''(E)$ as a function of temperature at (red circles) and below (blue squares) the resonance energy. The resonant peak appears below the superconducting transition temperature $T_c = 1.5$ K. Reprinted from Duan et al. 2021 [6] with permission from the authors. Reprinted with permission from Springer Nature, COPYRIGHT 2021.

Among the unique properties that make neutrons essential for probing quantum materials are their magnetic moment and corresponding magnetic scattering cross sections, which allow them to efficiently probe magnetic ground states and excitations in quantum materials. Their magnetic cross sections allow researchers to use elastically scattered neutrons to reconstruct how magnetic moments are ordered or correlated in quantum materials throughout a wide range of length scales reaching all the way to the atomic scale. The energy scale and corresponding wavelengths of the neutrons produced at SNS and HFIR make them unique for characterizing collective quantum states and their corresponding excitations. Neutron scattering allows researchers at these facilities to measure directly how much energy is required to create a quantum excitation in different materials as well as to determine how these excitations propagate through a material.

Because of these unique properties, neutrons will continue to play an important role in addressing the grand challenges of controlling material processes at the atomic scale, understanding and controlling correlated electron phenomena, and understanding emergence (when properties emerge from interactions between a manifold of constituent parts). Inelastic and elastic neutron scattering measurements of quantum spin liquids, topological materials, superconductors, quantum critical systems, quantum magnets, multiferroics, and systems with coupled degrees of freedom (lattice, electronic, spin, orbital) will be key to meeting these challenges and to advancing the quantum frontier of discovery-based research. Advanced computation and simulations giving access to state-of-the-art theory will be needed to model the complex behavior in real materials and interpret the measurement. Co-analysis with data from other complementary techniques will also be required.

Neutrons will continue to play an essential role in advancing the field of quantum materials. We also anticipate that neutron scattering will make important contributions in addressing priority research directions of national importance and urgent technological challenges. Two examples of such research directions, “Quantum Materials for Quantum Information,” and “Quantum Materials for Energy,” are described in the following subsections. These examples directly address important priority research directions identified in the DOE SC BES reports [7,8].

2.1.1 Example: Quantum Materials for Quantum Information

The goal of quantum information science is to advance communication and information processing by harnessing quantum entanglement and other quantum effects. Quantum entanglement uses correlations between atomic degrees of freedom to allow information to be encoded and processed in mathematically precise ways. This encoded information makes possible quantum communications, quantum computing, and quantum sensing. For all three applications, the ability to control quantum superposition and entanglement is essential. Materials that can encode, transduce, and process quantum information while maintaining quantum coherence are critical for achieving this goal. For example, quantum technologies will allow encoding of large volumes of information that exceed the information and processing capability of classical computers, so-called *quantum supremacy*, with mere hundreds of quantum bits (qubits). However, these qubits have stringent requirements. Quantum coherence must be maintained during computational operations, and the use of quantum error correction requires prohibitive overhead with current technologies.

Neutrons are an irreplaceable experimental resource with which to probe quantum states of materials and their quasiparticles, which carry the quantum information. As a quantum probe, neutrons characterize and quantify the entanglement in materials. Magnetism and superconductivity are primary phenomena associated with quantum entanglement in materials, and neutrons are a highly sensitive way to measure the quantum states of the electrons that give rise to these phenomena. Neutron scattering provides a unique energy and momentum-dependent probe of subtle aspects of quantum states via experiments on bulk materials.

The most compelling need is to find a quantum replacement for silicon. The electrons and holes that make classical computers work are quantum incoherent. Thermal fluctuations destroy any quantum information they may encode. Other materials can realize quantum quasiparticles that protect quantum information by tying the information in knots (i.e., protecting it topologically). Although such protection was only possible in principle a few years ago, it may be feasible in topological superconductors and quantum spin liquids. From these two classes of materials, different candidate materials that may provide topological protection of quantum information are being proposed.

Neutrons are essential to identifying topological superconducting and spin liquid materials with the non-Abelian quasiparticles that can implement fault-tolerant quantum computation. Capabilities needed to achieve fault-tolerant quantum computation include higher magnetic fields (15 T and larger) and low-temperature sample environments that will allow for tuning quantum systems into different regimes and to probe their underlying quantum states using neutron scattering. The high flux of continuous neutrons provided by the proposed MANTA instrument will enable crucial parametric studies as well as polarization tensor measurements to be undertaken that are currently difficult or impossible. The proposed MANTA instrument at HFIR, combined with cold neutron time-of-flight (TOF) spectrometer CNCS (BL-5) at SNS and the next-generation spectroscopy capabilities of CHESS at STS, will provide unprecedented complementary capabilities to probe complex quantum states and to extract their underlying Hamiltonians that enable detailed theoretical analysis of their properties. The highest fluxes that will be delivered by PPU and STS will be needed to undertake such experiments using the small single crystals that typically are available for the most exciting new materials. Further development of moderators and neutron detectors will enhance instrument performance when coupled with these improvements in source flux. Instrument upgrades at HFIR and SNS will further expand science opportunities to fully exploit the source improvements. Upgrades of PTAX (HB-1) and TAX (HB-3) at HFIR will provide a much-needed improvement of signal-to-noise to measure weak signals associated with quantum phenomena. Planned improvements in neutron polarization at PTAX (HB-1) at HFIR and HYSPEC (BL-14B) at SNS, including developments on neutron spin precession and spin-echo techniques will be essential to probe quantum entanglement. The combination of data analytics and simulations, for which the neutron data validate quantum simulations and computations of quantum states in materials, will provide a feedback loop for materials' codesign as well as for the development of quantum emulators and new quantum algorithms.

2.1.2 Example: Quantum Materials for Energy

Humankind has learned over centuries how to use materials and that, at the atomic-length scale, an underlying quantum world is responsible for the physical properties of materials. This quantum world comprises waves, interference, tunneling, fluctuations, entanglement, quasiparticles, and topology. Quantum materials, whose behavior is dominated by correlated electron physics or particles defined by charge, spin, and angular momentum degrees of freedom, can defy current limitations on energy transport and conversion. They hold promise for a next generation of high-speed low-power electronic technologies, as well as for energy conversion and transmission with improved efficiency and stability. Examples include topological semimetals for transmission without dissipation and low-power spintronics, efficient energy harvesting and fast photodetection, and superconductors through which electrical current flows with no resistance or energy loss. The interplay of correlations, symmetry, and topology drives and stabilizes exotic phases of matter and their excitations; when combined with theory and other advanced measurements, neutron scattering can provide the basic understanding of complex quantum materials and multilength and -timescale quantum phenomena to enable these applications.

Quantum materials are being considered for use in devices to improve energy efficiency; to reduce losses in power generation, transmission, and storage; and for improved sensor sensitivity and reliability. Quantum fluctuations, or the very small changes in energy associated with low-lying quantum states, are primarily caused by the interactions between electrons in a material. The collective behavior of these systems is sensitive to external perturbations on these correlated electrons. This sensitivity makes quantum materials candidates for use in a variety of devices. However, for any of these applications to become viable on a commercial scale, the fundamental behavior of quantum fluctuations must be understood. Neutron scattering fills this role in the study of quantum materials. Neutron scattering measurements of quantum materials provide detailed information of their dynamics and ordered phases down to the atomic scale.

Topological materials have surface properties that are significantly different than the bulk. These surface states are being considered for carrying large currents with little energy dissipation. Understanding the relationship between the bulk and surface states in topological materials as well as the dynamics and correlations at play in the surface states is a next step in making use of these exotic materials. Inelastic neutron scattering measurements can probe the magnetic excitations in topological magnon materials, allowing for examining details of the spectrum, such as Dirac points with linear band crossings for $CoTiO_3$, as shown in Figure 2.1-2.

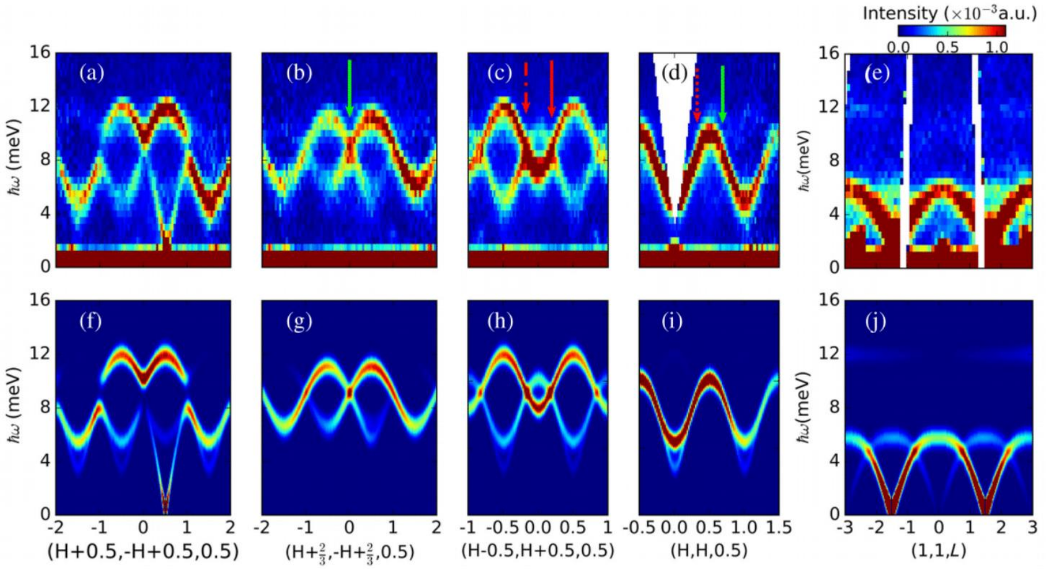

Figure 2.1-2. Magnetic excitation spectrum in the vicinity of the Dirac points as measured by inelastic neutron scattering using the SEQUOIA spectrometer (BL-17) at SNS (a–e) and the corresponding calculated (f–j) excitations. Neutron scattering measurements allow for quantitative comparison to the topological excitation spectrum. Reprinted from Yuan et al. 2020 [9] with permission from the authors and under the terms of the Creative Commons Attribution 4.0 International license**.**

Substantially improving speed and energy efficiency in computing and communications requires the ability to generate and control quantum effects near the atomic length scale. Quasiparticles all carry momentum and energy, but they also have properties of coherence, entanglement, and quantum transport. Producing and controlling these quasiparticles in devices requires fundamental understanding of their individual characteristics and how they interact and evolve. For example, magnetism can have large effects on the band structure of semimetals, driving transitions from Dirac to Weyl fermions and even to a topological insulating state. The energy scales of neutrons available at SNS and HFIR, as well as the magnetic moment of the neutron, make neutron scattering an especially useful probe of quantum materials for energy-relevant technologies.

Improved instrumentation of the thermal inelastic neutron scattering suites at HFIR and SNS will enable access to the electronic degrees of freedom, crystal fields, and higher energy interactions and correlations in topological superconductors and quantum spin liquids. Parametric studies in extreme magnetic fields (steady and pulsed) and high pressures will provide access to exotic field-driven states of matter and the nonthermal (in some cases quantum critical) transition between them. Specialized sample environments, including the highest magnetic fields, and spectrometers such as the proposed MANTA instrument at HFIR are required for understanding complex states and extracting their underlying Hamiltonians. The highest neutron flux that will be delivered by PPU and STS is needed to measure the signals from the correlated electron states responsible for the quantum properties. Development of moderators and neutron detectors will enhance instrument performance when coupled with these improvements in source flux, and ongoing instrument upgrades will expand science opportunities to fully exploit the source improvements. Advanced computation and simulations giving access to state-of-the-art theory will be needed to model the complex behavior in real materials and interpret the scattering data. Co-analysis with data from other techniques will also be required.

2.2 Soft Matter and Polymers

Soft materials, including polymers, colloids, surfactants, emulsions, liquid crystals, gels, nanocomposites, and more, are ubiquitous because their unique properties make them suitable for many applications. The development of novel soft materials requires an in-depth understanding of material structure–property relationships under different processing conditions. Neutron scattering has a strong history of contributing fundamental insights into soft matter and polymers not only because of the suitable length and energy scales probed but also because of the unique view that selective deuterium labeling affords in these hydrogen-rich materials.

For example, a recent experiment at the HFIR SANS (CG-2) provided essential structural information on a new type of heteropolymer in lipid bilayers that mimics the functionality of membrane proteins to transport ions across cellular membranes. In this study, transport measurements, spectroscopy, imaging, molecular dynamics simulation, and small-angle neutron scattering (SANS) were used to characterize the structure and function of the heteropolymers and their interaction with lipid bilayer membranes. This study showed that four-monomer-based random heteropolymers can mimic membrane proteins and exhibit selective proton transport across lipid bilayers at a rate like those of natural proton channels [10]. A key finding was that the segmental heterogeneity afforded by the four distinct monomers appears to be a key design feature that results in bilayer-spanning segments containing polar monomers that promote the formation of hydrogen-bonded chains that become “artificial channels” for proton transport. This process is illustrated in Figure 2.2-1.

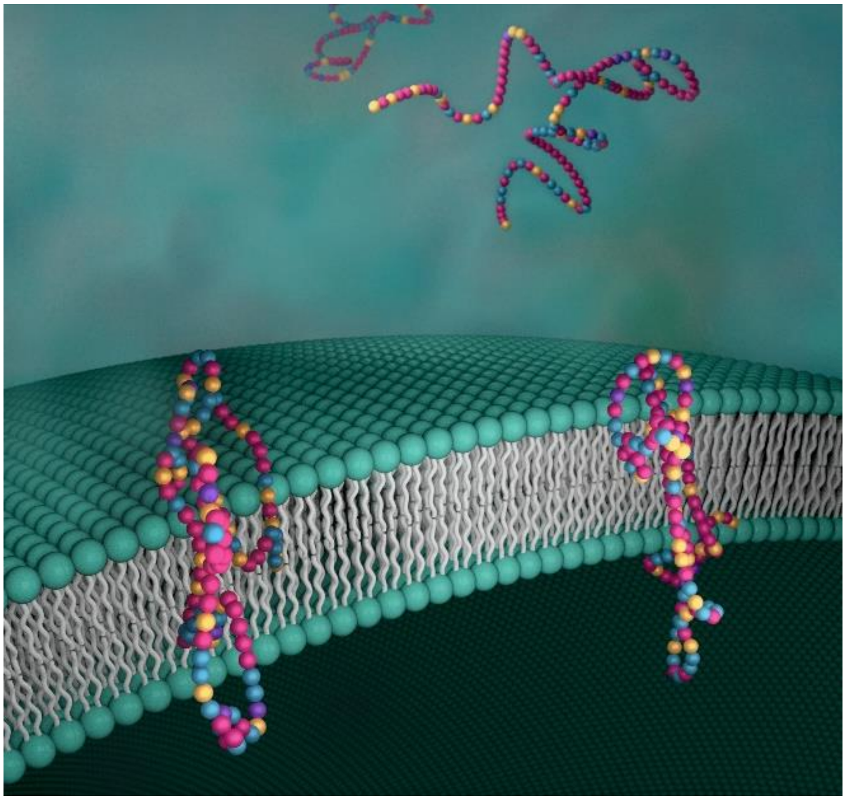

Figure 2.2-1. Artificial proton channels through membranes. The HFIR GP-SANS (CG-2) instrument provided essential structural information of random heteropolymers in lipid bilayers. The segmental heterogeneity afforded by the four distinct monomers appears to be a key design feature that promotes the formation of hydrogen-bonded chains that become "artificial channels" for proton transport across the lipid bilayer, mimicking the functionality of membrane proteins to transport ions across cellular membranes [10]. Illustration of the "artificial proton channels" (hydrogen-bonded chains) that transport protons across a membrane, (Credit: ORNL/Jill Hemman).

A characteristic feature of soft matter is nano- and mesoscale levels of morphology, which often are organized in hierarchical structures. These features are probed by large-scale structure neutron instruments, including small-angle and ultrasmall-angle neutron scattering beamlines, neutron reflectometers, and neutron imaging. Soft matter also exhibits a broad range of dynamic processes, metastable states, and low-energy interactions. The dynamics of soft matter is therefore studied by neutron scattering spectroscopy; motions are probed from the femtosecond timescale to approximately 100 ns, using inelastic neutron scattering, quasi-elastic neutron scattering (QENS), and neutron spin echo (NSE) instruments. Owing to the high penetrating power of neutrons, neutron scattering techniques are powerful for in situ/operando and multimodal characterization of soft materials under a variety of conditions. Moreover, isotopic labeling, together with solvent contrast variation, allows for studies of selective structures and dynamics of multiple component systems. This technique can highlight a component inside a sample by a specific labeling using isotopes, particularly hydrogen and deuterium, with drastically varying scattering length but minimum perturbation of the sample properties.

Because of their unique properties, neutrons will continue to be an essential tool in delivering important advances in soft matter investigations. Furthermore, they are anticipated to play an important role in use-inspired research that addresses the urgent technological challenges of delivering the clean-energy transition and ensuring environmental sustainability. In the following subsections, three examples of such use-inspired research are discussed: "Polymer Batteries," "Polymer Upcycling," and "Porous Soft

Materials for Capture, Separation and Storage of Greenhouse Gases.” These examples address important basic research directions and opportunities identified in the DOE SC BES reports [11,12].

2.2.1 Example: Polymer Batteries

The current demand and potential market growth for electrical energy storage (EES) in transportation, grid storage, and residential power-backup applications is of great interest because of the role it plays in clean energy. Fully realizing the potential of EES requires reduced cost and weight, higher energy and power densities, increased safety, improved lifetime, and environmental stability. These requirements will be met by using new EES device materials that have better chemical, electronic, structural, and mechanical properties that may be specific to the needs of the ultimate application.

Polymer batteries have unique benefits over traditional batteries that may allow them to fulfill energy storage needs for some applications. Polymer characteristics include ease of synthesis, low mass densities, chemical stability, low cost, compatibility with large-scale manufacturing processes, and mechanical stability. However, current polymer electrolytes suffer from poor ionic conductivity, high interfacial resistance, and poor oxidative stability. Bridging the critical knowledge gaps to realize the next generation of polymeric EES materials requires developing a predictive, multiscale, integrative understanding by using a combination of multidisciplinary experiment and theory.

Chemists and materials scientists are using a variety of techniques to develop new polymeric battery materials. Various strategies are being pursued that are both physical (plasticizers, inorganic fillers, polymer blending, and oligomer-tethered nanoparticles) and chemical (copolymerization, cross-linking, and the introduction of ionic side groups) in nature to design polymer electrolytes with the desired performance characteristics. NScD’s goal is to work with researchers who are creating new materials to understand the structure and dynamics at different time and length scales using neutron scattering methods. Neutron scattering techniques are ideally suited for developing an understanding of the correlation between the nanostructure and dynamics of these new materials and their electrochemical and mechanical performance. Neutron diffraction, SANS, and neutron imaging, which are already available at SNS and HFIR, can reveal the structures present at length scales from the interatomic to the macroscopic in battery materials. Neutron spectroscopies, such as NSE using SNS’s NSE (BL-15), QENS using BASIS (BL-2), and vibrational spectroscopy using VISION (BL-16B), reveal dynamics of the materials present.

For example, charge transport in a polymer electrolyte depends on the polymer hierarchical structure, chain segmental dynamics, salt concentration, and transport of all species at the length scales ranging from sub-nanometer to tens of nanometers, and it is not well understood. Nondestructive neutron scattering techniques combined with neutron contrast-matching methods and with other characterization techniques and simulation tools can provide predictive assessment of how to best optimize the facile transport of ions, mass, and heat in bulk electrodes and electrolytes and across electrode-electrolyte interfaces under applied potentials. Neutron scattering is imperative to probe the morphology of polymer electrolytes, the kinetics of ions, the dynamics of segmental movements, the phonon coupling with ion motion and heat transfer, and the transport of ions and atoms at and across electrode-electrolyte interfaces. Recently Chen et al. [10] employed QENS to investigate the segmental motion of polyethylene oxide (PEO) chains under the confinement of LiTFSI salt and Ohara ceramic. This study shed light on how to engineer the surface chemistry to enhance the ionic conductivity of polymer electrolytes (Figure 2.2-2). STS’s high peak brightness and lower repetition rate will allow access to subsecond resolution of kinetics for in situ experiments and hierarchical structure from the atomic to molecular scale (0.1–100 nm). For example, the future CENTAUR instrument at STS will provide unprecedented dynamic range in length scales probed simultaneously. Similarly, EXPANSE, the future high-resolution NSE instrument at STS, will provide access to information not presently available from other instruments at

ORNL. The knowledge gained will inform new material developments and theory to explain performance. Artificial intelligence (AI) and machine learning (ML) methods will be required to integrate all the information and to reveal relationships not readily evident from a single experimental technique that cannot provide a complete picture of the material by itself. Combined, the effort will lead to a predictive understanding and the next generation of EES materials.

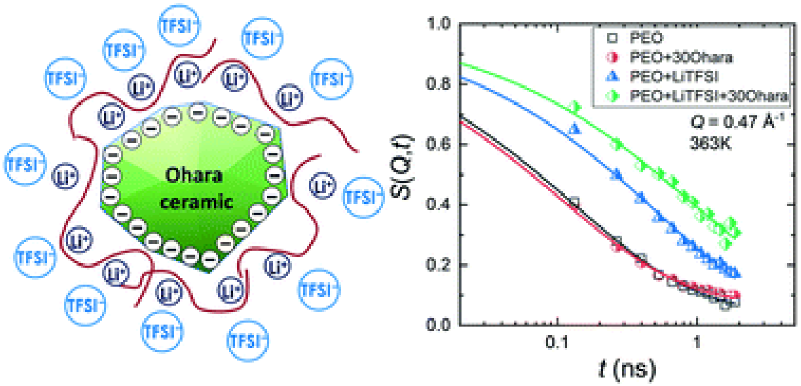

Figure 2.2-2. Polymer segmental dynamics obtained by QENS advances understanding of the ion transport in a ceramic polymer electrolyte. (left) Schematic representation showing ion distributions on the ceramic–polymer composite; (right) Intermediate scattering function *S*(*Q*, *t*) as a function of time, *t*. Reprinted from Chen et al. 2019 [13] with permission from the authors. Copyright the Royal Society of Chemistry 2019, permission from the Royal Society of Chemistry conveyed through Copyright Clearance Center Inc.

2.2.2 Example: Polymer Upcycling

The world produces over 380 million tons of solid plastic every year, and only approximately 9% of those are currently recycled. Solid plastic recycling is a grand challenge. Conventional approaches, such as mechanical recycling, are insufficient to address the growing accumulation of discarded plastics. The challenge is to develop a new path for upcycling plastics. Foundational knowledge is needed to design new chemical reactions, catalysts, processes, and materials that enable efficient deconstruction, reconstruction, and functionalization of discarded plastics into higher value products. Gaining this knowledge depends on in situ and operando characterization methods combined with real-time computational modeling, simulations, and data analytics to uncover the mechanisms and kinetics of deconstruction, reconstruction, and separations.

Neutron scattering techniques are exquisite for in situ/operando characterization of polymeric materials under extreme and/or processing-relevant conditions. The appropriate sample environments that mimic the conditions inside polymer processing equipment all the way through injection and deposition can elucidate how to manage these materials. The kinetics of crystallization; the size, shape, organization, and entanglement of chain molecules; the interaction of compatibilizers at the interface between noncompatible materials; and the dynamics of reversible bonds (as foreseen to be extremely relevant in the new generation of polymeric materials) can all be studied in detail using neutron scattering techniques, particularly when combined with selective isotopic labeling to highlight components in blended materials that are impossible to investigate with any other technique. Owing to neutrons' nondestructive and penetrating properties, in situ studies of these materials under realistic processing conditions are possible with the right sample environments, and the time and spatial resolution of such studies will greatly benefit from the future high-flux neutron source at STS. Neutron scattering methods are essential to provide unique information. For example, in situ analysis of the products of depolymerization under supercritical fluids facilitate the development of value-added materials while addressing the challenge of plastic waste. Similarly, the interaction of compatibilizers with the mixed streams of plastic waste can be interrogated using neutron scattering techniques, providing key information about the deconstruction and repolymerization of these materials.

Inelastic neutron scattering methods provide critical information on polymer dynamics across a wide range of length and time scales, from local dynamics using QENS to the slow nanoscale dynamics probed by NSE. These techniques, when combined with structural studies and computer simulations, can enable in silico design of advanced materials. The future HFIR NSE, with the capability of covering a broad *Q*-range and Fourier time of 400–500 ns routinely (700 ns maximumly), will enable probing smaller sample volumes and higher throughput measurements. These experimental measurements, complemented by coarse-grained molecular dynamics, will provide benchmark datasets for evaluating supervised ML algorithms.

Polymers with reversible (dynamic) bonds (e.g., vitrimers) are generating new interest because they present easily recyclable polymers with unique properties, such as self-healing, time-programmable behavior, extreme toughness, and extensibility. Understanding the dynamics of polymers that take place from picoseconds to hundreds of nanoseconds with reversible bonds can provide key information to optimize the processing conditions for upcycling. EXPANSE, the future wide-angle NSE at STS, will advance the understanding of collective dynamics simultaneously on the scale from angstroms to 100 nm. The neutron imaging technique offers the promise that the behavior of multicomponent systems, such as those resulting from a mixed waste stream, can be studied in situ in polymer-processing equipment without the need for deuteration. The penetration power of neutrons allows crucial insights into events inside injection molds and extruder screws, providing crucial information about the effects of compatibilizers. Labs equipped with traditional characterization capabilities (e.g., x-ray, differential thermal analysis, dynamic mechanical analysis, differential scanning calorimeter, rheology) will be extremely useful for the ex situ sample examination of the online upcycling measurements.

2.2.3 Example: Porous Soft Materials for Capture, Separation, and Storage of Greenhouse Gases

Rapid climate change is a grand challenge, and soft materials have unparalleled potential for efficient capture, separation, and storage of greenhouse gases to contribute to net-zero carbon emissions by 2050. Among these materials, covalent organic frameworks and metal organic frameworks have been the subjects of intense research efforts throughout the last decade because of their large capture capacity, high selectivity, tunable pore size, and easy pore functionalization. However, their poor stability and performance underwater and under acidic conditions significantly limit their applications.

The design of novel materials with improved performances requires atomic/molecular-level understanding and control of gas–host structure, kinetics, and dynamics, especially at the relevant diverse conditions such as pressure and temperature. Neutron scattering methods, owing to neutrons’ high penetrating power and isotope (particularly hydrogen/deuterium) labeling, present exciting opportunities to provide foundational insights into the intrinsically heterogeneous structure, complex interactions across multiple length scales, and slow dynamics of soft materials and guest molecules selectively in them. Furthermore, neutron scattering methods offer the capability to bridge the understandings of microscopic origins of macroscopically observed behaviors across a large span of time and length scales in situ/operando. In turn, this knowledge will provide insights into the design of improved soft materials with the desired fine-tuned functional properties.

Neutron elastic scattering techniques can make important contributions to understanding the effects of pore size, size distribution, pore connectivity, and interfacial structure, as well as topology on the gas capture and separation under operating conditions (Figure 2.2-3). The dynamics of the confined molecules (i.e., gas, water, and ions) can be measured with QENS. The dynamics of soft materials are often collective/cooperative, involving many structural units. However, in contrast with single-particle motions, these collective dynamics are poorly understood. The collective dynamics in soft matter can be studied using coherent neutron scattering (e.g., NSE), consequently providing an estimate of the characteristic length scale of cooperativity and dynamic heterogeneity. Understanding how cooperative motions change under confinement, especially when the confinement size approaches the length scale of dynamic cooperativity/heterogeneity, is the key to controlling the diffusion of gas molecules through the porous soft systems.

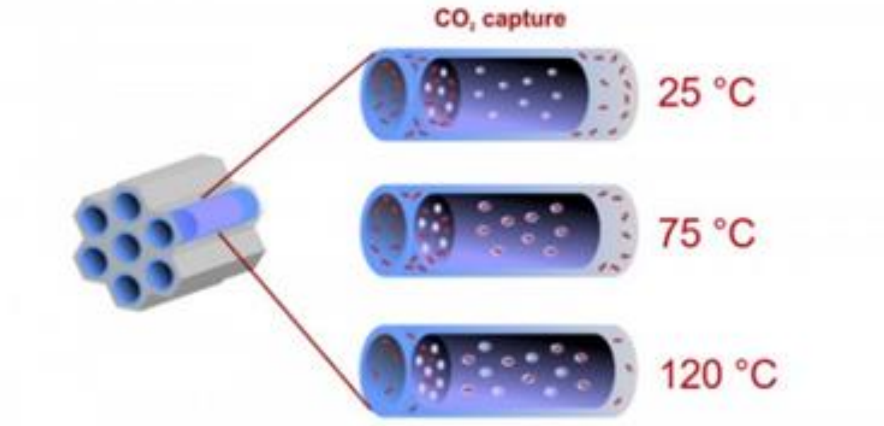

Figure 2.2-3. SANS measurements provide essential information to optimize CO_2 capture conditions. (left) structure of Santa Barbara Amorphous (SBA)-15/polyethylenimine (PEI)-50, mesoporous silica (grey) highly loaded with surface (blue) and volume (purple) PEI. (right) Volume PEI exhibits voids (light dots) that expand above 75°C. CO2 molecules (black C, red O) physisorbed on mesopore surface. for SBA-15/PEI-50 the optimal temperature for CO2 capture is 75°C. Reprinted from Zhang et al. 2019 [13] with permission from the authors. Copyright 2019 American Chemical Society.

Advances in neutron imaging have enabled spatial resolution of the accumulation of gas molecules inside porous media. Currently, valuable information about dynamic gas trapping processes can be obtained in 2D, and advanced reconstruction algorithms and time-lapse tomography could potentially monitor the dynamic gas trapping processes in 3D. However, the temporal and spatial resolution must be improved to capture the movements and location of confined gas molecules in more detail, which depends on the development of multifaceted parameters including neutron detectors, optical components, and neutron source characteristics (Section 3.2.4). Experiments on well-characterized systems can provide useful input to computer simulations, which are essential to obtain gas capture/separation/storage information of complex porous systems that experiments alone cannot provide.

Consequently, neutron scattering, coupled with molecular simulations, is expected to provide essential information toward the understanding of the structure/dynamics/reactivity in soft materials' host systems. This understanding will facilitate the design of robust and innovative porous soft materials for gas separation, capture, and storage.

2.3 Materials and Engineering

Materials are at the heart of technologies, devices, and the societal infrastructure that will define the future US economy and provide solutions to present and future challenges in many areas, including energy, transportation, communications, and security. The road from discovery of fundamental scientific principles to implementation of new concepts and materials design is long. The ability to rapidly characterize materials is essential to accelerate their discovery and application. Therefore, efficient approaches must be found to create materials' underlying new technologies. Characteristics of novel materials must be understood under relevant operating conditions, including functionality, reliability, degradation, and failure mechanisms over time in service. Neutrons have unique properties that make them crucial for the characterization of novel materials.

For example, a recent experiment at the VULCAN (BL-7) instrument at SNS revealed how a new aluminum–cerium (AlCe) alloy behaves under the high temperatures and pressures inside an operating internal combustion engine [10]. The penetrating power of neutrons provided noninvasive measurement of lattice strains inside components of a firing engine, enabling the operando study of complex load states and thermal gradients throughout the solid materials. For this experiment, the researchers fitted an AlCe cylinder head to a commercial engine typically used in construction and industrial applications (Figure 2.3-1). The resultant measurements were then related to microscopic stresses, enabling a comparison of the stress distribution between the experimental cylinder head and the original engine block during different stages of the engine's operation. The research demonstrated the superiority of a cerium-rich alloy in maintaining structural integrity and provided key data to further advance the alloy development. This approach can be used to aid research on advanced alloys for future engines and other systems.

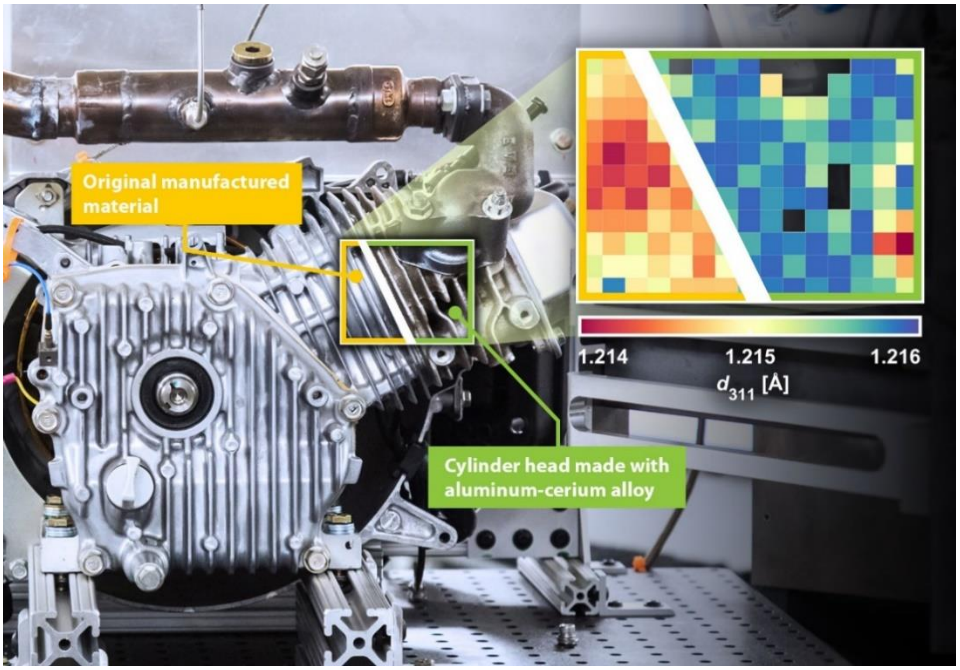

Figure 2.3-1. Real-time diagnostics for better engines. Neutron diffraction was used to investigate a new aluminum-cerium (AlCe) alloy's behavior under the high temperatures and pressures inside an operating internal combustion engine [15]. Analysis of the color map of the measured atomic spacings allows for comparison of the original material (left) and a new, experimental high-performance aluminum-cerium alloy (right). [Credit: ORNL]

Neutron scattering is one of the rare tools that can reveal time-resolved and energy-dependent responses of matter in practical configurations under extreme and complex conditions. This information is critical to the discovery and development of new structural, functional, or energy materials, as well as new processing parameters that directly affect people's daily lives. A deeper structural understanding can enable (1) the creation of more stable and efficient ferroelectric, piezoelectric, and thermoelectric materials for future consumer electronics; (2) more effective and selective catalysts that are less susceptible to poisoning; and (3) new high-entropy alloys and oxides with a range of desirable functional properties. Example themes are mechanical and physical properties of advanced alloys and ceramics; structure and performance of materials by advanced manufacturing; structural integrity of engineering components and matters in harsh environments, such as irradiation damage in nuclear reactor support structures; and using disorder and high entropy to create new functional materials. The goals are to shorten the time required to develop and validate new materials, thereby bringing them to market sooner; to characterize materials under real-life operating conditions; and to extend the service life of critical engineering structures.

Neutrons provide unique multiscale nondestructive penetrating probes of crystallographic or morphological structures in bulk materials and structures by using diffraction, SANS, and imaging. Specialized neutron techniques, such as spatially resolved engineering diffraction and imaging contrasts at the multilength scale, complement many other advanced characterization tools for a wide range of engineering, structural, and smart materials. Neutron instruments can be designed to accommodate large and complex sample environments, including radioactive materials chambers, real devices, and industrial components to study the synthesis process, microstructure, and a material's physical and chemical properties during or close to the manufacturing process. The structure or property of physical and/or chemical materials (like atomic disordering, ordering, pair distribution, elasticity, twinning, nucleus, cluster, precipitate, phase transformation, residual/internal stress, hardening, softening, stacking faults, dislocation density, void, crack, and distortion) are investigated to understand materials' design–structure–property–performance relationship by using neutrons under standalone or combined mechanical, thermal, electrical, chemical, magnetic fields in lab or application scale.

Neutrons will undoubtedly continue to be an essential probe in the pursuit of new and better materials, and they will make enormous contributions to solve materials challenges of national importance. The following subsections describe two examples of such challenges: "Transformative Manufacturing," and "Materials for complex reactor environments." These examples address important research directions identified in the DOE SC BES reports [16,17].

2.3.1 Example: Transformative Manufacturing

Neutrons are critical for elucidating the coupled underlying physical and chemical events across scales in additive manufacturing of large structures during process. Directed-energy deposition additive manufacturing adds to-be-melt feedstock at the same time as the heat input, involving rapid nonequilibrium and complex chemical and physical changes into the built structures. The defects that develop during this extreme process (e.g., voids, impurities, distortion, residual stresses) affect the material-dependent mechanical and structural integrity of the built structures. Postprint processing is often required to address these deficiencies. Understanding the fundamental science of the additive manufacturing processes is essential to innovating materials and to processing strategies that will enable first-time-right transformative manufacturing [15]. The goal is to understand the coupled underlying physical and chemical events across scales in additive manufacturing processes and products via AI/ML-assisted neutron scattering and to integrate multiphysics models and tools to inspire materials design and to enable adaptive manufacturing control.

Large operando manufacturing tools can be developed to fit on the neutron instruments (e.g., the additive manufacturing system in Figure 2.3-2) to study the physical and chemical properties of materials or structures under conditions that emulate manufacturing processes. Neutron characterization of these materials provides a science-based understanding of factors that arise during transformative manufacturing, such as complex multiple time and length scales; nonequilibrium phenomena and mechanisms, including phase transformation; buildup of defects or dislocations; texture; and residual stress. Nondestructive postmortem measurements by engineering diffraction mapping and imaging tomography reveals internal characteristics in complex-built structures. Using the high-fidelity data produced from operando direct-energy deposition, additive manufacturing on large neutron experimental facilities can elucidate without ambiguity the formation pathways of matter under extreme states to discover the manufacturing synthesis–structure–property–performance relationship, identify critical influences on system performance, provide an effective path to validate multiphysics models, and bridge the gap between modeling and applications.

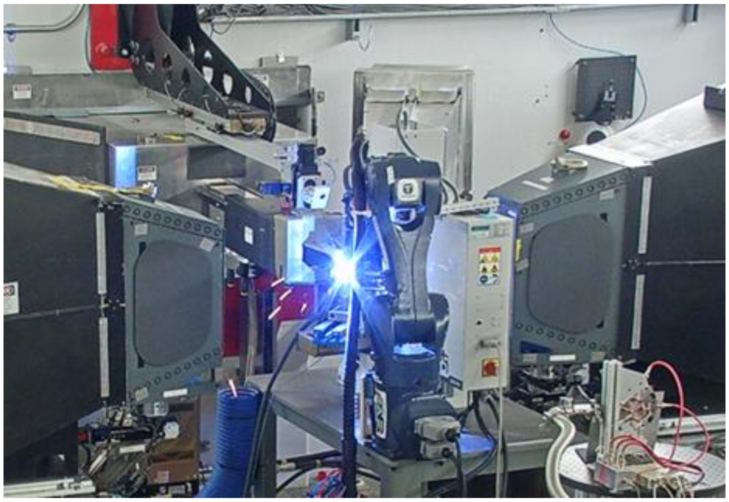

Figure 2.3-2. Neutron facilities can host large processing devices for materials operando studies. As shown in the photo, ORNL is demonstrating a robot arm equipped with wire arc welding on VULCAN (BL-7) at SNS to enable operando nondestructive neutron diffraction measurement of phase transformation and buildup of residual stress in a structure during additive manufacturing. (Credit: ORNL)

The combination of the higher neutron flux provided by the SNS PPU; increased detector coverage at instruments; multimodal measurements; and live analysis algorithms, including AI/ML methods, will enable high-fidelity, in situ mechanical, physical, and microstructural scientific understanding of materials across atomic scales, nanoscales, and mesoscales to facilitate in-process decision-making and adaptive control with fast surrogate models on high-performance computers. This new understanding of processing and materials response can be used to identify the key aspects that are detrimental to desired built structure properties to design a suitable materials system for direct-energy deposition additive manufacturing.

2.3.2 Example: Materials for Complex Reactor Environments

Harsh and complex nuclear reactor environments involving heat, stress, corrosion, and radiation require durable materials to ensure a long-term energy supply with reliable performance and safety. A basic research need exists to uncover the fundamental science understanding of the chemical process and materials responses cause the degradation in properties and loss of performance that affect the fuel, coolant, and structural materials in complex reactor environments [17]. Neutrons can help advance the understanding of nuclear materials by investigating complex physical, structural, and chemical evolutions under extreme external stimuli. In addition to typical stimuli (e.g., temperature, pressure, and stress), understanding the material’s response to radiation is extremely important. The goal is to advance the radiolytic understanding of nuclear materials under extreme stimuli, enabling nuclear materials exploration and optimization for next-generation nuclear reactor design.

Given the unique way neutrons interact with high-*Z* materials—especially with nuclear fuel materials—neutron scattering and imaging techniques play a significant role in nondestructively characterizing traits such as heterogeneity and defect in solid or liquid fuel. Furthermore, neutrons in epithermal range (>1 eV) show abrupt changes (a few orders of magnitude) in cross section, known as absorption resonance, when interacting with certain nuclei, which are isotope specific. These characteristics provide unique contrast in resolving spatial distributions at an isotopic level when combined with TOF neutron imaging (Figure 2.3-3) at spallation neutron sources, such as the VENUS instrument (under construction).

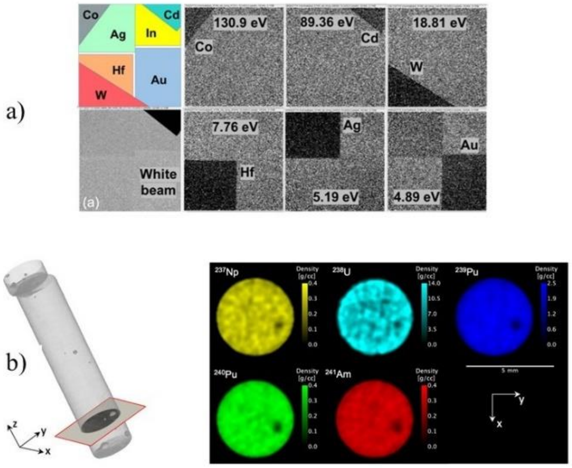

Figure 2.3-3. Energy-resolved neutron imaging is a powerful nondestructive technique to characterize materials for complex reactor environments. (a) Neutron radiographs obtained at labeled resonance energies that highlight each element in a stack of metallic foils. Reprinted from Zhang et al. 2018 [18] with permission from the authors. Copyright 2018 by the American Nuclear Society, La Grange Park, Illinois. (b) Neutron tomography of a nuclear fuel material, U-20Pu-10Zr-3Np-2Am, collected using epithermal neutrons at a pulsed source. Slices normal to the cylinder axis are shown with corresponding isotopes and densities labeled. Reprinted from Losko and Vogel 2022 [19] with permission from the authors and under the terms of the Creative Commons CC BY license.

Besides being a powerful scattering probe in obtaining chemical and structural information, neutrons' high penetration through typical radiation shielding enables the studies of irradiated materials such as fuel cladding, spent fuel, and coolant. Although these studies are challenging for other state-of-the-art techniques, neutron scattering techniques are well positioned to provide insights into materials' physical and chemical evolutions under the complex and harsh reactor environments across multiple time and length scales. Combining such characterization with in-house development of AI/ML algorithms will provide improved understanding of nuclear materials' complex and linked underlying physical and chemical processes that lead to degradations in nuclear material, including structural materials and coolants [17]. This understanding contributes to the knowledge base and accelerates material discovery, design, and optimization for future nuclear energy applications.

2.4 Chemistry and Environmental Sciences

Modern life depends on chemical processes and reactions to provide essential compounds used as components for commodity and specialty products, including plastics, functional materials, batteries, electronics, and building materials. Modern life also relies heavily on hydrocarbons sourced from oil, natural gas, and coal extraction, and understanding the "cradle-to-grave" journey of raw materials, materials recycling, and energy efficient manufacturing has become a necessity. At the same time, devices are becoming increasingly more compact, while battery cycle times and storage are expected to dramatically increase. New and better materials must be developed to fill this need, and better chemical processes must be found that lower the environmental impact on atmosphere, water, and soil. Neutrons' sensitivity to hydrogen and their ability to penetrate deeply inside materials make them ideal to explore and to obtain new insights into the performance of novel materials and chemical processes. For example, recent experiments at VISION (BL-16B), combined with total scattering measurements at NOMAD (BL-1B) and DFT on a novel metal catalyst used to convert nitrogen into ammonia, revealed that the catalyst's primary reaction mechanism occurs because of the catalyst's surface hydrogens, not those encaged inside the metal as previously believed [20] (Figure 2.4-1). This discovery paves the way for further studies to optimize the catalyst's potential for higher performance. The novel catalyst used in this study—made of ruthenium, calcium, and aluminum—catalyzes ammonia with significantly less energy (heat and pressure) than the traditional iron-based catalysts.

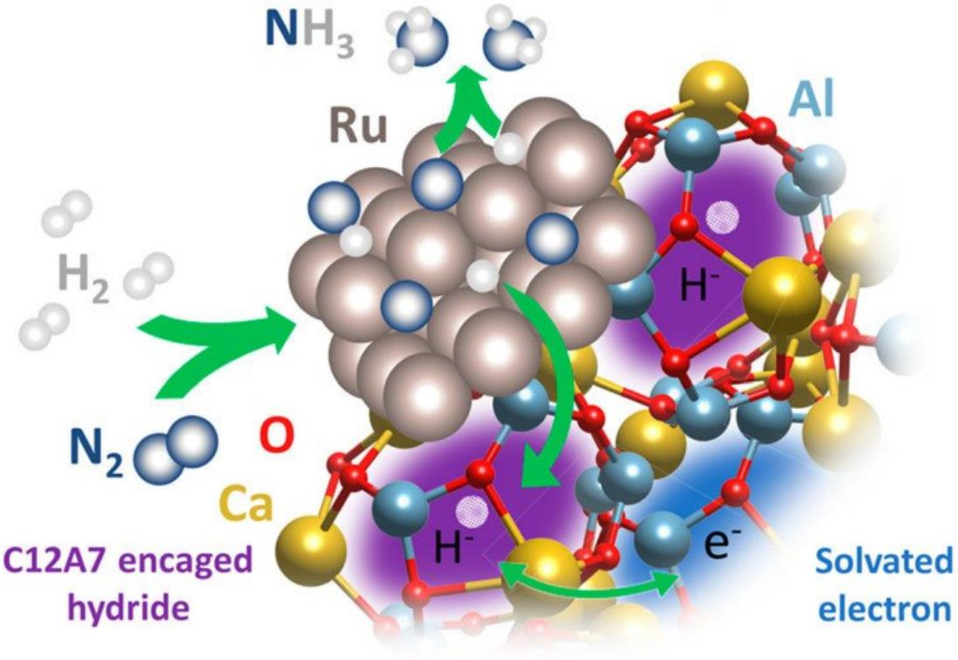

Figure 2.4-1. Novel catalyst enables ammonia synthesis with less heat and pressure. The atomic structure of the ruthenium-calcium-aluminum metal catalyst used in ammonia synthesis. A recent neutron scattering experiment, along with computer modeling, showed that the hydrogen atoms on the surface react with nitrogen atoms to form ammonia. The novel catalyst uses considerably less heat and pressure than other catalysts. Reprinted from Kammert et al. [20] with permission from the authors.

The user facilities at HFIR and SNS provide a range of techniques to investigate unstructured materials—amorphous liquids, solids, powders—up to highly structured crystalline materials. Diffraction can be used to characterize long-range and short-range structures, bonding arrangements, and energies. Surface- and interface-binding energies, diffusion, and chemical fingerprinting are being studied by using quasi-elastic scattering and chemical vibrational spectroscopy. SANS provides important local structure information at the nanoscale. Reflectometry determines the neutron scattering length–density–depth profile in interfaces, yielding a composition–depth profile.

In addition to this neutron scattering instrumentation, in operando environments that probe time-dependent behavior under alternating conditions to capture away-from-equilibrium and intermediate states are often needed decipher reaction kinetics. Therefore, complex experimental setups are needed to simultaneously vary selected stimuli of temperature, pressure, gas environment, magnetic fields, current and voltage, and light to mimic real-world processing conditions and adequately drive material behavior. Specifically, using cycling and alternating conditions, stroboscopic and pulsed experiments will allow access to more extreme conditions and will enable probing nonequilibrium conditions. The goal is to be able to routinely slice the collected data according to the varying parameters in the metadata on the fly and use the visible trends as feedback for experiment steering. Molecular- and atomic-level simulations are also needed for detailed modeling of the data, and, in some cases, high-performance computing (HPC) will be needed.

Neutrons' unique properties will allow them to play an essential role in the study of new materials and chemical processes. They will also play an important role in addressing the urgent technological challenges of delivering the clean energy transition and ensuring environmental sustainability. The following subsections present three examples of such technological challenges: "Hydrogen Economy and Catalysis of Green Ammonia," "Carbon Cycle, Carbon Dioxide Capture, Conversion, and Storage," and "Batteries/energy storage and conversion." These examples address important priority research directions and opportunities in the DOE SC BES reports [11,21–24].

2.4.1 Example: Hydrogen Economy and Catalysis of Green Ammonia

Currently, most of the energy economy is anchored to fossil fuels based on hydrocarbons as an energy-storage medium. After centralized refining, fossil fuels are ready for transport to the end consumer without further modifications. However, fossil fuels are a precious nonrenewable resource, and hydrocarbon consumption produces various environmentally harmful by-products. Alternative, nonhydrocarbon-based energy storage solutions include solid-oxide fuel cells, flow batteries, flywheels, compressed-air energy storage, and pumped hydropower. However, these alternatives often require energy-intensive processing but provide only low energy density storage. A promising alternative is an economy based on hydrogen storage in which the energy is stored in chemical bonds. Although this approach is not yet on the commercial horizon, chemical energy storage has several advantages over conventional solutions. First, forming stable chemical compounds that can be reacted to release the energy stored in the bonds provides a stockpile of energy for later use. Second, chemical storage could achieve high energy density when the compounds are in liquid or solid form. Energy stored in chemical bonds has higher density than other available energy resources. Finally, this approach allows the stored energy to be transported to on-demand consumers. Thus, chemical hydrogen batteries are an appealing alternative to conventional batteries in terms of efficient energy storage.

One important step toward making chemical energy storage a practical reality is the demonstration of an environmentally friendly chemical battery for hydrogen storage by generating ammonia from water and air using a hydrocarbon-free catalysis process. This process engages the two most readily available molecules on the planet, water and nitrogen gas as starting materials to produce ammonia as an energy-storage medium for high-density energy storage of hydrogen. Ammonia has the advantages of having high hydrogen density and of being amenable to liquefaction and storage, which facilitates transportation. Ammonia is currently produced with the aid of catalysts, in particular ferrous catalysts, as used in the Haber–Bosch process, an environmentally harmful, resource-intensive industrial process. The solution to this problem is to tune and develop novel catalysts that can produce ammonia from surface water and nitrogen from air and to use catalysts to decompose ammonia into hydrogen and nitrogen in a multistep process.

The ammonia/nitrogen cycle, illustrated in Figure 2.4-2, could be a zero-carbon emission technology, consuming only three abundant elements with the aid of green energy and new catalysts. To produce the hydrogen from water, electrolysis is necessary to break down the water molecule. With the hydrogen from water and the nitrogen from air, ammonia can be produced catalytically. The goal is to employ catalysis pathways of co-electrolysis of water and nitrogen gas to eliminate the energy-intensive and pressure-assisted thermal catalysis common to the Haber-Bosch process. Furthermore, the ammonia can be stored as liquid (low pressure) and in solid form (i.e., in amine compounds [25]); it can also be adsorbed in porous materials [26,27].

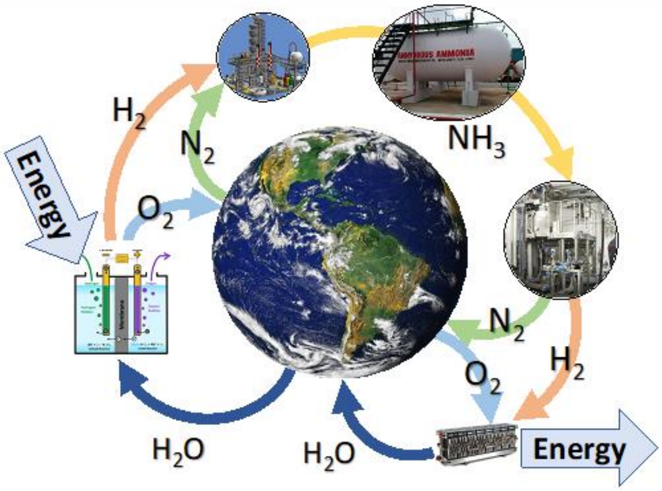

Figure 2.4-2. Illustration of the ammonia/nitrogen cycle. Natural surface water from the environment (e.g., sea, lake, river) is electrolyzed to produce hydrogen and oxygen, preferably using renewable energy. Oxygen may be returned to the atmosphere, and hydrogen is further reacted with nitrogen from air to produce ammonia. Ammonia can easily be stored and transported to the point of use. Ammonia can be decomposed into nitrogen and hydrogen; hydrogen is used to produce energy with oxygen extracted from air. The only by-product of this cycle is water.

To recover the stored energy, hydrogen can be produced from the decomposition of ammonia using catalysts to run fuel cells, gas turbines to produce electricity, and other energy applications. Storing energy for future use is a matter of strategic importance (supply stability) because most renewable sources are intermittent. Neutrons, with their unmatched sensitivity to hydrogen, are ideal in pursuit of the development of an ammonium battery and can be used in most stages of this process, including hydrolysis, catalysis, solid-state chemistry, and breaking the N–N bond. For example, recent in situ neutron scattering measurements at VISION (BL-16B), combined with total scattering measurements at NOMAD (BL-1B) and DFT calculations [20], have revealed that surfaced-adsorbed hydrogen, rather than hydride encaged in a catalyst electride, plays an important role in ammonia synthesis (Figure 2.4-1). Thus, neutron scattering can lead to a better understanding of the mechanisms of ammonia synthesis, leading to more efficient catalysis for many difficult hydrogenation reactions. The higher neutron fluxes provided by the SNS PPU combined with the planned developments in neutron moderators, new detector technologies, sample environments for in situ measurements, and advanced modeling and simulations are needed to make significant contributions in this field.

2.4.2 Example: Carbon Cycle, Carbon Dioxide Capture, Conversion, and Storage

The world’s reliance on fossil fuels for commodity chemicals, transportation fuel, and materials manufacturing presents serious challenges to society. Chemical cracking and burning of hydrocarbon-based fossil fuels produces the potent greenhouse gas CO_2, which traps heat in the atmosphere, causing global warming. The CO_2 produced by hydrocarbon fuels is often admixed with SO_2 and NO_x gases, which are also harmful to the environment. Finding ways to reduce and remove CO_2 from the environment is thus an endeavor with high societal impact.

Because of its low chemical reactivity, CO_2 is not a coveted reagent. Its conversion to value-added products, such as formic acid, methanol, fuels, or other feedstock for the chemical industry, is challenging. Furthermore, achieving a carbon-neutron cycle is difficult because CO_2 is released during the individual production processes of intermediate and end products. Another challenge concerns the capture of CO_2, which is often present in low concentration in the atmosphere or in gas streams from chemical operations. Separation and purification of CO_2 from gas streams typically require energy-intensive treatment to separate and concentrate CO_2. Various schemes have been proposed, but the development of materials and processes with high efficiency and low energetic costs remains a priority [28]. Finally, if CO_2 is to become a commodity for the chemical industry, then efficient and low-cost storage of purified CO_2 that is directly usable by industrial processes will require R&D. Further investigation of geological storage underground in depleted salt domes or oil fields and conversion to future accessible carbonates is a development field for geochemistry and environmental science.

Neutron scattering can be used in developing materials to address CO_2 capture in three main categories: (1) materials for the physical or chemical capture of CO_2, (2) catalysts to lower the energetic cost needed to break down CO_2 chemically, and (3) functionalized or advanced porous materials for selective gas separation. Although promising materials are being studied in the laboratory, practical problems remain. Neutron vibrational spectroscopy, diffraction, QENS, inelastic neutron scattering, SANS, and reflectometry are specifically well suited to measure the catalytic efficiency of zeolites for CO_2 conversion. Zeolites are functionalized with metal centers (alternatives to currently used platinum group metals or rare earth elements) to facilitate achieving acceptable efficiencies and process conditions that minimize energy, resources, and waste, as well as support a circular economy concept. Chai et al. demonstrated catalytic separation of mixed alkynes and olefines with high chemical selectivity by large-pored zeolites, incorporating active individual copper and nickel sites [29]. Direct CO_2 capture from air in the solid state is developing as a promising alternative to wet methods, and neutrons are ideal tools with which to study this process because of their sensitivity to light elements and their penetrating power, as illustrated by a recent experiment at TOPAZ (BL-12) [30].

New approaches to catalytic selectivity require the understanding of more complex systems, enabling mild process conditions to minimize environmental impact. For example, hybridized metal organic frameworks combined with ionic porous organic frameworks have been proposed and studied for CO_2 separation and conversion. These frameworks can incorporate functional metal sites and activate CO_2 while maintaining the porosity of hybrid materials, thereby improving the mass transfer rate and catalytic efficiency [31]. Neutron scattering can play an important role in the search for efficient, self-regenerating, low-impact, chemically stable, selective catalysis systems. Significant discoveries in this scientific area will require the continued improvement of the current instrument suites at SNS and HFIR. The PPU, the HBRR, and the pressure vessel replacement (PVR) will increase the capability of the current instrument suite by delivering higher fluxes. The planned developments in neutron moderators at SNS, new detector technologies, sample environments for in situ operando measurements, and advanced modeling and simulations are needed to make significant contributions in this field.

2.4.3 Example: Batteries/Energy Storage

Simultaneously maximizing energy density and rate capability in batteries is the obvious conundrum to inspire the next generation of increasingly compact energy storage devices. This challenge is fundamental for energy storage, which calls for basic research breakthroughs to make qualitative advances in electrochemical cells [32]. Neutron scattering is uniquely capable of probing the transport of molecular and ionic species that govern the charge transfer in electrochemical devices. Neutrons are well suited for investigating structural and dynamical properties of materials in the angstrom to micron length scales and the sub-picosecond to hundreds of nanoseconds timescales. Neutron scattering also provides well-known advantages for these investigations, such as hydrogen/deuterium contrast matching, quasi-elastic scattering of hydrogenous compounds, greater sensitivity to lithium in heavy metal matrices in elastic scattering than in x-ray scattering, sensitivity to lattice dynamics, and magnetic/electronic transitions/energy levels.

Current energy storage research focuses on phase stability, ion motion, defects, local structures, and site occupancies in the crystalline phase of battery materials under variable temperature and gas environments. These environments may have diffraction and scattering density variations that arise from liquid phase-change formation. For example, Jafta et al. [33] recently used operando SANS measurements to show how the use of a concentrated electrolyte in Li/ordered mesoporous carbon half cells influences the mechanism of solid electrolyte interphase formation, lithium intercalation, and carbon framework expansion. This study demonstrated that operando SANS is a unique method for providing microstructure and composition dependent information on the dynamics of electrochemical processes in batteries.

Extending the operando studies of electrolytes for longer range correlations and rheological effects as well as to failure mechanisms will go a long way toward improving electrochemical batteries to meet future demands. Influential discoveries in this area will require the continued improvement of the current instrument suite at SNS and HFIR. The PPU, the HBRR, and the PVR will increase the capability of the current instrument suite by delivering higher fluxes and allowing the measurement of weaker signals. Molecular- and atomic-level simulations are also needed for detailed data modeling. To make full use of the neutron scattering capabilities at HFIR and SNS will require the development of a sample environment platform that enables operando electrochemical capabilities that are readily interchangeable among neutron scattering instruments to perform measurements in charging-discharging operation. The formidable challenges of these studies include significant technique-dependent variability and the need to measure the scattering signal specifically from the anode, electrolyte, or cathode, and their interfaces, one at a time.

2.5 Biological Materials and Systems

Understanding the molecular basis and organizational complexity of life remains an outstanding twenty-first century scientific challenge and will be fundamental to advances in bioenergy sciences, bioremediation, defense, human health, and medicine. To meet this challenge, modern molecular and structural biology relies upon the integration of knowledge from multiple techniques and modalities that provide mechanistic and functional insights across multiple levels of organization. Imaging technologies underpin and inform much of this research, providing detailed structural and dynamical information on macromolecular systems and biological processes at the atomic, molecular, and cellular levels of detail. Neutron scattering provides distinctively detailed information about the structure and dynamics of biomaterials and systems across length scales that range from 1 to 10,000 Å and timescales that range from femtoseconds to nanoseconds. Specifically, neutron scattering uniquely contributes to the understanding of how macromolecules work, interact, and combine into cells' functional complexes, hierarchical assemblies, molecular machines, and membrane-associated components.

For example, a recent experiment at the SNS-MANDI (BL-11B) and HFIR-IMAGINE (CG-4D) instruments located the position of the hydrogen atoms in the main protease (3CL M^{pro}) from SARS-CoV-2, the agent of COVID-19 [34] (Figure 2.5-1). The 3CL M^{pro} from the SARS-CoV-2 virus is an essential enzyme for viral replication, and inhibiting it prevents the virus from replicating. Thus, understanding its structure is an important step in the design and development of SARS-CoV-2 specific protease inhibitors and for repurposing existing clinical drugs to combat SARS-CoV-2. The full structure was determined by jointly refining x-ray and neutron diffraction data; the neutron data allowed for visualization of the protonation states and the hydrogen bonding. The fine atomic details present in this structure were revealed by the unique scattering properties of the neutron, which is an ideal probe for locating hydrogen positions and experimentally determining protonation states at near-physiological temperature. This important result s provides critical information for structure-assisted and computational drug design, enabling precise tailoring of inhibitors to the enzyme's electrostatic environment.

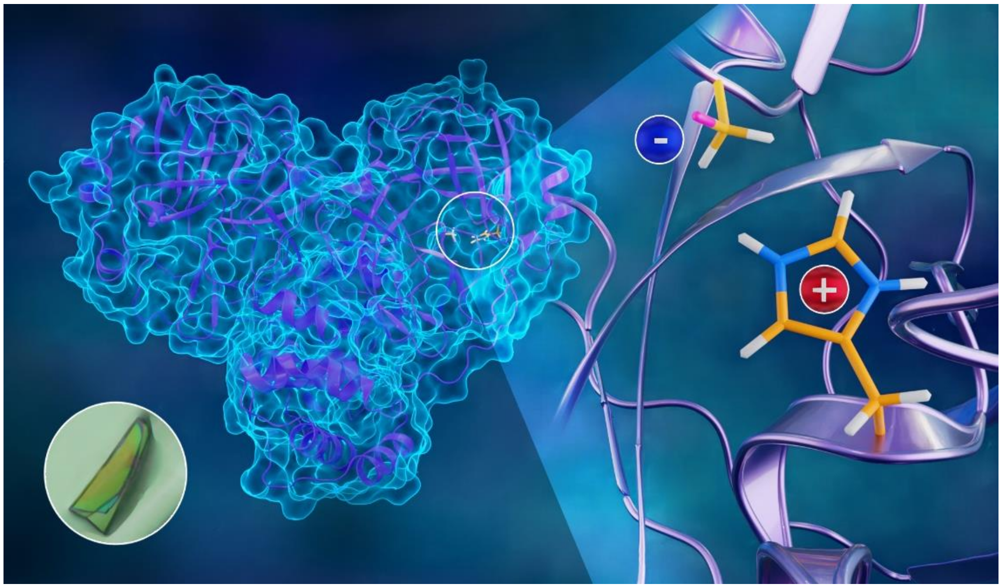

Figure 2.5-1. Mapping hydrogen atoms in SARS-CoV-2 main protease. The image shows the SARS-CoV-2 main protease crystal used in a recent neutron diffraction experiment by Kneller et al [34] (left), the enzyme molecule in cartoon representation with transparent surface (center), and a zoomed-in area on the catalytic site (right), illustrating the negatively and positively charged residues. Credit: ORNL/Jill Hemman.

Neutron scattering is exquisitely sensitive to hydrogen atoms in biological materials. It provides a unique, powerful, and nondestructive tool for the analysis of structure–function and interfacial relationships across multiple levels of organization. Moreover, neutrons, in contrast to probes routinely used in biology such as x-rays or electrons, scatter differently from hydrogen and its deuterium isotope. Therefore, in mixed systems, individual components can be selectively labeled with deuterium to determine and highlight their atomic position, global structure, or dynamics. Targeted applications encompass atomic resolution analysis of individual hydrogen atoms in enzymes via mesoscale and macroscale analyses of complex biological structures, substrates, scaffolds, membranes, or assemblies of interest to energy, environment, defense, health, and medicine. These unique features guarantee that neutrons will continue to play an important role in the advancement of biological materials and systems.

At the atomic level, neutron diffraction provides structural information of biological systems, including the location of individual hydrogen atoms. SANS probes interactions within protein complexes and hierarchical assemblies, providing understanding of long-range regulation processes such as allostery. Neutron reflectometry allows for characterizing membranes and biologically relevant thin films and interfaces. Neutron spectroscopy provides information about the underlying molecular motions and dynamical behavior of biological materials.

Bioscience research interests are broadly defined by the structure and dynamics of biological assemblies. Influential discoveries in biological materials and systems will require the continued improvement of the current instrument suite at SNS and HFIR. The development of sample environments (Section 3.4.1) enabling in situ and operando experiments will open new opportunities for translational science. Additionally, the new instrument VENUS will open new opportunities in the field of medical imaging.

Neutrons will continue to play an important role in the field of biological materials and systems. They are also likely to make significant contributions toward addressing major technological challenges of national importance. The following subsections describe three research examples that address the technological challenges of the clean energy transition and environmental sustainability: “Nature-Inspired Catalysis: Understanding and Redesigning Enzymes with New or Improved Properties and Functions,” "Plant Cell Walls and Microbial Systems for Advanced Biofuels and Bioproducts," and "Bioinspired Memristive Membranes Capable of Machine Learning." These examples address research directions and opportunities outlined in the DOE BES, BER and EERE reports [12,21,22,24,35,36,37,38,39].

2.5.1 Example: Nature-Inspired Catalysis: Understanding and Redesigning Enzymes with New or Improved Properties and Functions

Neutron scattering can facilitate (1) understanding and harnessing the chemistries and design rules that enzymes use to catalyze reactions in living systems and (2) inspiring development of new classes of catalysts engineered to function and perform in less harsh industrial environments. The challenge is to identify bioinspired catalysts that will function under less extreme temperatures, pressures, and pHs to reduce the energy costs and environmental impacts of industrial processes.

Fundamental to this goal is understanding how nature can use common base metals (e.g., iron, copper, manganese) organized within transient organic scaffolds (proteins) to fix nitrogen (nitrogenases), split water, generate hydrogen, and break down (and repurpose) complex waste streams and materials, all at room temperature and in aqueous solution. To answer this, we must determine the molecular designs and processes that enable living systems to capture, transfer, convert, and store solar/chemical energy. These investigations will inspire the development of new classes of catalysts and devices that operate under near-ambient conditions and that are custom designed to power and support a sustainable energy future.

Understanding and harnessing the chemistries and design rules that enzymes use to catalyze reactions in living systems require probing enzymes beyond the active site. Neutron scattering techniques across several time and length scales provide important means to probe the structure and dynamics of the extended environment of the enzyme's active site. Neutron diffraction enables the location of individual hydrogen atoms and the chemical nature of intermediates to be determined at the active site of metalloenzymes without driving redox chemistries. SANS probes interactions within protein complexes and hierarchical assemblies, providing understanding of long-range regulation processes such as allostery. Although the role of dynamics—of the protein itself and its environment (solvent)—in the regulation of enzyme activity has been established, neutron spectroscopy provides information about the underlying molecular motions and dynamical behavior of enzymes. Industrial applications may require an enzyme to be immobilized or tethered on surfaces, neutron imaging can be used to characterize these support materials, and neutron reflectometry describes the distribution of the tethered enzyme on surface.

The PPU (Section 3.1.2) and the HBRR and PVR (Section 3.1.4) will increase the capability of the current suite of instruments by delivering higher fluxes, thereby enabling the measurement of smaller samples. Suitable sample environments must be developed to recreate industrial setups (i.e., extreme pH, pressure, temperature) (Section 3.4.1) to understand how these parameters affect enzyme structure and dynamics and, consequently, activity. The development and implementation of dynamic nuclear polarization (Section 3.5.2.4) together with advances in sample-labeling techniques (Section 3.4.5), detector technologies (Section 3.5.1), and data acquisition, reduction, and analysis (Section 3.3) will allow for analyzing samples that cannot currently be measured. The advanced imaging capabilities of the future VENUS instrument will open new opportunities to characterize enzymes on support surfaces needed for industrial applications.

2.5.2 Example: Plant Cell Walls and Microbial Systems for Advanced Biofuels and Bioproducts

The conversion of biomass to biofuels and valorization of non-fermentable components to bioproducts and engineering microbes with higher efficiency are important scientific missions of the DOE SC Biological and Environmental Research (BER) program [37-38]. Synergistically, the DOE Office of Energy Efficiency and Renewable Energy (EERE) and the DOE SC BES program support research focused mechanistic understanding of the plant cell wall assembly and commercialization of bioproducts from plant cell wall polymers [39]. These investments seek to understand the hierarchical complex structure of the plant cell wall during its assembly and deconstruction, and development of efficient engineered microbial systems for producing biofuels and bioproducts.

Investigating the molecular organization of biomass and the structural changes that occur during its deconstruction is an active area of research in the Neutron Scattering Division in partnership with the Biosciences Division under a BER funded Bio-Fuels Science Focus Area project. This project is closely aligned with the Center for Structural Molecular Biology (CSMB) and regularly uses BIO-SANS (CG-3) at HFIR for this research [40,41]. In addition, the success of this project has given rise to an independent user community that use neutron scattering for characterization of cellulosics and related bioproducts [42,43]. A central thematic area is understanding how biomass structure changes during thermochemical deconstruction. To date, we have employed an empirical approach by correlating changes in cell wall structure to the efficiency of a particular pretreatment regime. We propose to extend this approach to develop a predictive understanding of the relationship between pretreatment conditions with the structural changes observed by SANS. This will be achieved by developing beam-line automation to improve measurement throughput and execution. It will be coupled with the development of AI computational methods to determine which key observations from SANS can be correlated with solvent combinations and pretreatment conditions that will result in optimal sugar release for biofuels of efficient separation of polymers for bioproducts production. Related to this research we will expand our deuteration capabilities to produce deuterated precursors for selective deuteration of cell wall polymers in planta. Combining selective deuteration with advances in genetic engineering of plants provides a means to probe the intricate and complex interactions between cell wall polymers in their native environment to obtain a better understanding for the design rules for the synthesis, assembly, and hierarchical organization of plant cell walls. This understanding will enable us to take advantage of the unique capabilities of neutron scattering by allowing the structure of individual cell wall components to be observed in their native environment. This type of information cannot be obtained by other techniques. As an enabling technology for this work, we will develop new data analysis tools for interpretation of 2D SANS images. This capability will increase the fidelity of our models and help to extract higher fidelity structural information from SANS than is currently possible.

The microbial systems used for conversion of pretreated biomass to biofuels and other bioproducts are often inhibited by pretreatment by-products and alcohols such as ethanol and butanol that they produce during fermentation. Understanding the inhibition mechanism for destabilization of these organisms is crucial for efficient production of biofuels. Alcohols produced during fermentation are known to disrupt plasma membrane function, but the underlying mechanism is poorly understood. Neutrons are ideally suited to studying the structure and dynamics systems providing information about membrane thinning, phase separation of lipid classes, modulus changes, lipid diffusion, and/or increasing permeability that can be detrimental to cell integrity or to hinder membrane associated protein function with slower and/or reduced efficiency. Judicious use of deuterium labeling techniques for in vitro or in vivo neutron scattering studies will help understand the location and molecular flexibility of different alcohols within the biomembrane, especially with different types (length, saturation, etc.) of lipids. These studies will ultimately contribute to the development of more robust membranes that can counter the effects caused by solvents for the improvement of biofuels production.

This research requires the development of automation for sample environments as well as the development of biological and chemical synthetic approaches for deuterated biomolecules (Section 3.4.5). The PPU (Section 3.1.2) and HBRR (Section 3.1.4) will benefit experimental capabilities by providing increased flux and improved guide systems, respectively. New approaches for data acquisition, reduction, and data analysis (Section 3.3.3) will facilitate measurements that are currently difficult or not feasible.

2.5.3 Example: Bioinspired Memristive Membranes Capable of Machine Learning

Circuit elements capable of storing information in analog form without needing power will revolutionize computing and elucidate the principles that underpin learning and memory in the human brain. Two-terminal mem-elements (e.g., memcapacitors, memristors) with nonlinear electrical behavior offer the possibility of collocating memory and signal processing to produce the next generation of computers capable of emulating the brain's efficiency and flexible cognitive capabilities. Lipid bilayers have the potential to be developed into neuromorphic platforms with tunable plasticity and diverse functionality—if they can demonstrate both learning and long-term memory.

Neutron scattering can help develop and understand the design rules for a new class of recyclable energy-efficient self-assembled memristors composed of biomembranes that possess the key features needed to make neuromorphic computing and sensing a reality. The challenge is to identify biomemristors that operate at significantly lower power consumption levels compared with currently available solid-state technologies. Importantly, these biomolecular devices will emulate key synaptic functions and will enable brain-like learning and computing tasks when configured in neuromorphic circuits. This effort will require the combination of neutron scattering and AI/ML strategies to enhance the performance of both the individual devices and the highly distributed networks of brain-inspired neuromorphic sensors with advanced communication abilities.

Of the major classes of biomolecules (i.e., lipids, proteins, nucleic acids, and carbohydrates), membrane lipids are the richest in hydrogen and are thus readily detected and easily distinguished from the others. Importantly, hydrogen/deuterium isotopic labeling provides dramatic improvements in sensitivity and selectivity in scattering experiments and obviates the need for chemical tags and their associated artifacts. Neutron reflectometry can be used to determine the 1D scattering length density along the bilayer normal with nanoscale resolution and the in-plane structure under various device working conditions (Figure 2.5-2). Using neutron reflectometry, the membrane can be characterized while performing in situ measurements that impart memory and learning to the device. Interrogating different parts of the membrane separately requires developing novel sample environment and deuteration schemes.

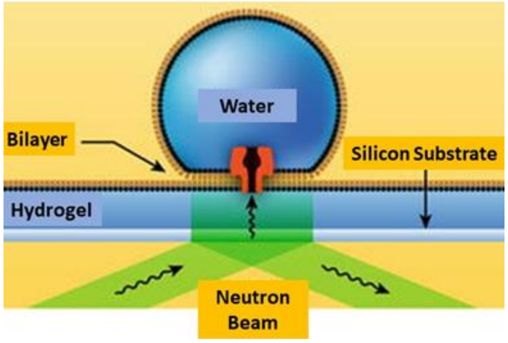

Figure 2.5-2. Schematic of in operando characterization of neuromorphic devices using neutron reflectometry.

Currently, compelling evidence exists for learning in single cells that lack a nervous system and for which the mechanisms underpinning popular theories for learning and memory—memory engram cells and synaptic plasticity—both have lipid membranes in common. Lipid membranes are currently being considered as essential for synaptic plasticity and memory formation. Moreover, direct electrical stimulation of the brain has therapeutic effects on neurological and a wide range of neurocognitive disorders via mechanisms that are currently unknown. The ultimate goals are (1) to develop and fabricate a new class of energy-efficient memristors composed entirely of biomolecules as a platform for the next generation of neuromorphic computers and (2) to explore the lipid bilayer as a novel therapeutic target where certain types of memory are stored in the human brain.

Performing this research requires the development of novel sample environment and deuteration schemes that will enable different parts of the membrane to be interrogated separately. Higher neutron fluxes provided by the PPU (Section 3.1.2) will enable the measurement of smaller samples. Developments in detector technologies (Section 3.5.1) and in data acquisition, reduction, and analysis (Section 3.3) will enable analyzing samples that cannot currently be measured.

These R&D areas will drive development of the infrastructure, tools, and expertise that will be needed for the facility, its staff, and the research community to achieve these goals.

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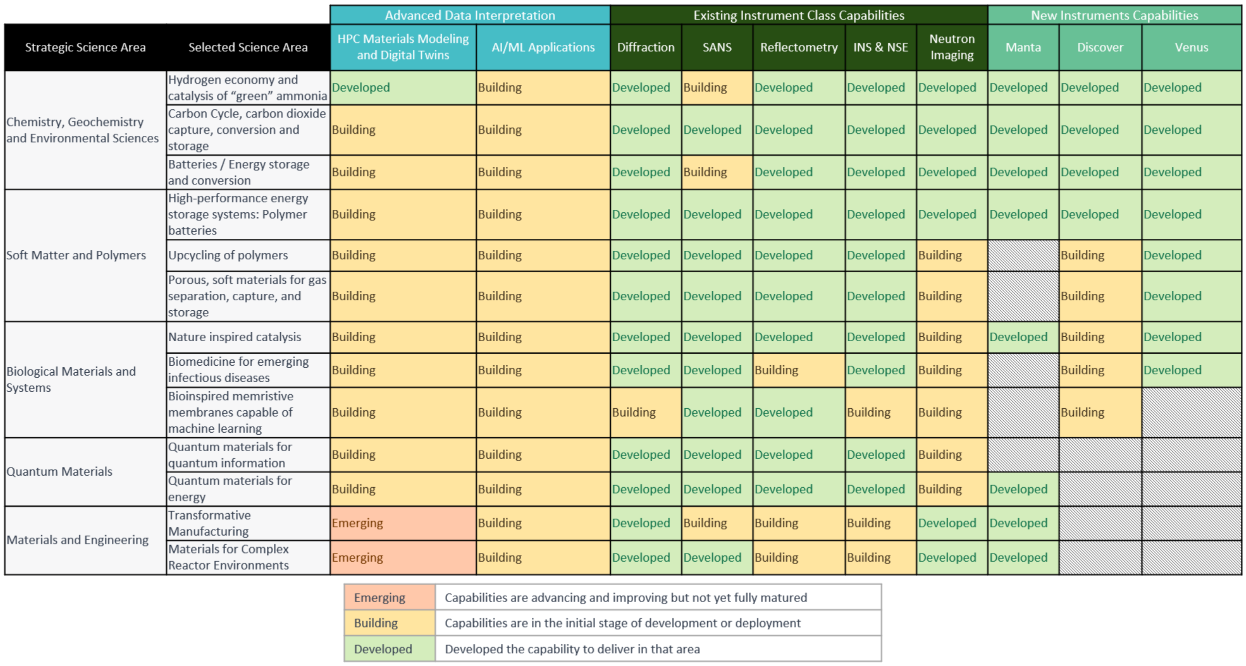
3 TECHNICAL CAPABILITIES AND DEVELOPMENTS

The *10-Year Strategic Plan for Neutron Sciences* aims to establish a direct link between the planned technical developments and investments and the science areas that we seek to impact (Section 2). The strategic planning process involves establishing directions regarding existing and new neutron sources and instrumentation, technological developments, software, sample environments, and operations that will ensure that we are ready to meet the science challenges and national needs of the future.

In this section, we present our vision on how to accomplish this work. We present our outlook on the future of our neutron sources; plans for instrumentation improvements and upgrades; plans for new instrumentation; developments on data acquisition, reduction, and analysis; and plans for sample environments; as well as anticipated technological developments. Special care was taken to ensure that each element of this vision can be linked to one or more of the strategic science areas and examples are illustrated in Table 3.1.

Table 3.1. Technological development needs by strategic science areas and highlighted examples.



		Advanced Data Interpretation		Existing Instrument Class Capabilities					New Instruments Capabilities		
Strategic Science Area	Selected Science Area	HPC Materials Modeling and Digital Twins	AI/ML Applications	Diffraction	SANS	Reflectometry	INS & NSE	Neutron Imaging	Manta	Discover	Venus
Chemistry, Geochemistry and Environmental Sciences	Hydrogen economy and catalysis of "green" ammonia	Developed	Building	Developed	Building	Developed	Developed	Developed	Developed	Developed	Developed
	Carbon Cycle, carbon dioxide capture, conversion and storage	Building	Building	Developed	Developed	Developed	Developed	Developed	Developed	Developed	Developed
	Batteries / Energy storage and conversion	Building	Building	Developed	Building	Developed	Developed	Developed	Developed	Developed	Developed
Soft Matter and Polymers	High-performance energy storage systems: Polymer batteries	Building	Building	Developed	Developed	Developed	Developed	Developed	Developed	Developed	Developed
	Upcycling of polymers	Building	Building	Developed	Developed	Developed	Developed	Building	▨	Building	Developed
	Porous, soft materials for gas separation, capture, and storage	Building	Building	Developed	Developed	Developed	Developed	Building	▨	Building	Developed
Biological Materials and Systems	Nature inspired catalysis	Building	Building	Developed	Developed	Developed	Developed	Building	Developed	Building	Developed
	Biomedicine for emerging infectious diseases	Building	Building	Developed	Developed	Building	Developed	Building	▨	Building	Developed
	Bioinspired memristive membranes capable of machine learning	Building	Building	Building	Developed	Developed	Building	Building	▨	Building	▨
Quantum Materials	Quantum materials for quantum information	Building	Building	Developed	Developed	Developed	Developed	Building	▨	▨	▨
	Quantum materials for energy	Building	Building	Developed	Developed	Developed	Developed	Building	Developed	▨	▨
Materials and Engineering	Transformative Manufacturing	Emerging	Building	Developed	Building	Building	Building	Developed	Developed	▨	▨
	Materials for Complex Reactor Environments	Emerging	Building	Developed	Developed	Building	Building	Developed	Developed	▨	▨

Emerging	Capabilities are advancing and improving but not yet fully matured
Building	Capabilities are in the initial stage of development or deployment
Developed	Developed the capability to deliver in that area

Last, but not least, we present our vision on operational excellence, which includes workforce development; diversity and inclusion; work-life balance; the user program; communication strategy; environment, safety, health, and quality (ESH&Q); and asset management. These areas are all essential to operate our facilities and to run a world-class-neutron scattering program that meets the science challenges and national needs.

We then close this section with a high-level 10-year schedule of this plan's implementation.

3.1 Neutron Sources, 10-Year Outlook and Beyond.

Although the timeline for this plan is 10 years, there are important efforts that must take place in the near future in order to impact the future of our facilities beyond 10 years. STS, currently under design, will provide capabilities that complement the capabilities of the SNS First Target Station (FTS) when it is completed between 2032 and 2037. The combination of the pulsed neutron capabilities of the SNS FTS, STS, and the steady-state thermal and neutron beam capabilities at HFIR will place NScD in a world-leadership position in neutron scattering research.

This section presents an outline of the three-source strategy [1], including current efforts to upgrade and improve SNS and HFIR. The PPU Project is in progress at SNS, and the HBRR at HFIR is planned for 2028. Both efforts are accompanied by improvements and opportunities. Finally, a recent report of a subcommittee charged with assessing the scientific justification for a US domestic high-performance reactor-based research facility [2] recommended the replacement of the HFIR pressure vessel to extend its life for another 50 years or more. This recommendation has prompted ORNL to plan for new future opportunities for HFIR.

3.1.1 The Three-Source Strategy

NScD develops and operates two world-class neutron user facilities that provide researchers with advanced neutron scattering capabilities. SNS is the world's highest power pulsed neutron source, providing intense beams of neutrons in short bursts at its FTS with a 60 Hz repetition rate. HFIR provides the brightest steady-state thermal and cold neutron beams. The new SNS STS project will provide a third source that complements the inherent technical strengths of the current sources as summarized:

- SNS FTS—high repetition rate, high resolution, focused bandwidth, thermal, and epithermal neutrons
- SNS STS—high peak brightness of cold neutrons, large bandwidth, small beams
- HFIR—high time-integrated flux for both cold and thermal neutrons, polarized neutrons, focusing monochromators

A relevant figure of merit for sources like SNS is the peak brightness at specific neutron wavelengths, which is a measure of the number of useful neutrons produced in a single pulse of the source. For a continuous source of neutrons, the companion figure of merit is the average brightness, which measures the total number of useful neutrons produced per unit time at specified wavelengths. Figure 3.1-1 shows peak and average brightness of the ORNL neutron sources in comparison with other world-class neutron sources at neutron wavelengths of 1 and 5 Å. In combination, these three sources will provide the diversity and flexibility to provide world-class neutron scattering capabilities to the US research community. These three technically diverse sources provide the platform to adapt to changing science needs and will ensure US leadership in neutron sciences for decades to come.

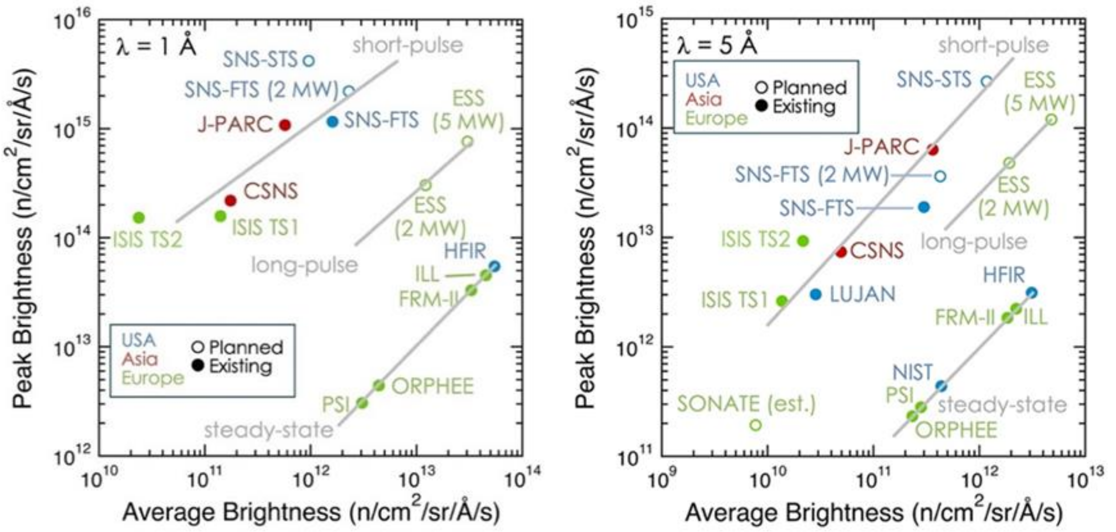


Figure 3.1-1. Peak and time-averaged brightness of current (closed circles) and planned (open circles) neutron sources. Illustrated at neutron wavelengths of (a) 1 Å and (b) 5 Å.

Three ORNL Neutron Sources

The three-source strategy [1] outlines the means by which NScD will deliver a vision of maximum scientific impact across the three sources at HFIR and SNS while enhancing the technical flexibility needed to adapt to evolving science demands. Key to this strategy is to place all neutron instruments at the source that maximizes their performance and to maintain investment in the sources and instrument suites to provide US researchers continued access to world-class neutron scattering capabilities. As envisioned, the following elements of this strategy for each of the sources is an approximately 20 year vision.

- SNS FTS
  - Complete, upgrade, and renew the instrument suite.
  - Redesign and then replace the moderator-reflector plug to respond to expected changes at STS and HFIR, replacing the coupled moderators with fully optimized high-brightness moderators and realigning the instrument suite to the key strengths of the FTS.

- SNS STS
  - Build STS and its associated initial instrument suite, taking full advantage of the recent development of high-brightness parahydrogen moderators.
  - Design and construct more instruments to fully populate all available beam ports with world-leading instruments designed to take full advantage of STS’s key strengths.

- HFIR
  - Continue to strengthen the thermal and cold neutron instrument suite, replacing the existing guide network as part of the HBRR Project.
  - Replace the pressure vessel as part of a lifetime extension project. The new vessel should incorporate redesigned beam tubes and a new reflector assembly, which would allow the instruments to reach world-leading performance while realigning the instrument suite to play to the key strengths of the neutron source.

  - Improve illumination of the cold guide system by increasing the size of the cold source and/or allowing close-proximity guides, feeding an upgraded suite of cold-neutron instruments in the guide hall.
  - Build a new thermal-neutron guide hall with a new suite of world-leading, low-background instruments.

More details are provided in the following sections on the parts of this vision that are planned within the approximate 10 year time frame of this document.

3.1.2 The SNS First Target Station, Proton Power Upgrade

The SNS FTS produces neutrons at a relatively high repetition rate of 60 Hz and 1.4 MW. SNS came online in 2006. Its technical design was established in the 1990s as the first of a pair of next-generation megawatt-class pulsed spallation neutron sources; the other is in Japan (J-PARC). SNS is the highest-power spallation neutron source in the world and provides correspondingly world-class performance for its instrument suite. SNS capabilities have increased dramatically since it first came online. The initial suite of 3 instruments has been expanded to 18 instruments for materials science as well as a fundamental physics beamline. The accelerator has increased from an initial power level below 100 kW to a steady 1.4 MW today while also routinely meeting or exceeding the 90% design reliability metric. The instrument performance has also greatly improved; many of the most significant changes relate to improvements in instrument control, data acquisition and reduction software, sample environment equipment, and increases in detector coverage.

The key feature of short-pulse spallation sources is their very high peak neutron brightness. As the highest-power spallation source in the world, SNS provides the highest peak brightness, particularly for high resolution and short wavelength applications. Its key technical strengths can be summarized as follows:

- High peak brightness—For thermal and epithermal neutrons, the peak brightness is the highest in the world. For many instruments using the TOF technique, peak brightness is the key factor determining instrument performance. Many of the instruments at SNS are therefore world-leading in performance.
- High resolution—The short neutron pulses arising from the design of the decoupled and poisoned moderators translates directly into high resolution in both reciprocal space and energy.
- Focused bandwidth—With a repetition rate of 60 Hz, the high peak brightness combines with a measurement bandwidth that, although large compared with that of reactor-based instruments, is intentionally narrower than at any other pulsed spallation source. Thus, it can deliver data in the specific volume of reciprocal and energy space where it is needed.

The advent of the SNS STS and the expectation of improved performance at HFIR provide an opportunity to plan more broadly while benefitting from the substantial operational experience on FTS. The following areas are open for improvement:

- The original FTS design requirement to serve the widest possible range of neutron applications resulted in compromises in the moderator brightness, particularly for the cold coupled moderators. The key technological breakthrough for STS will be the performance of its cold coupled moderators.
- The FTS design was finalized in the 1990s and represents the state of the art at that time. Since then, significant advances have been made not only in moderators but also in critical instrument technologies. The expected lifetime of an instrument is typically 20 years before it is eclipsed by technological change and evolving scientific trends, although a major upgrade can extend it by 10 years or so. Given that the first FTS instruments are now 15 years old, the instrument suite is no longer fully state of the art.

- Most, but not all, of the FTS beam ports have now been populated with instruments. Projects are underway or are being prepared to build instruments on two of the five remaining available beam ports.
- A few FTS instruments still have sizeable gaps in their detector coverage or other well-identified paths for significant upgrades.

The PPU Project will involve upgrading the SNS accelerator complex to double the currently available proton beam power from 1.4 to 2.8 MW while retaining the 60 Hz repetition rate. Upon project completion in 2024, the PPU will be capable of delivering 2 MW to the SNS FTS. Operations at 2 MW, which will result in an urgently needed increase in flux that will enable new scientific discoveries in the five strategic science areas described in Section 2, will start in 2026 after a gradual and planned power increase. The PPU will enable experiments that currently are not feasible or routine, such as time-resolved in situ measurements, experiments on smaller or less concentrated samples, and experiments under more extreme environmental conditions [3].

3.1.3 The SNS Second Target Station

The SNS STS project will build a second target station at SNS. The new source will operate at 700 kW with a 15 Hz repetition rate, taking one out of every four proton pulses produced by the PPU-upgraded SNS accelerator. STS will complement the technical strengths of the other two ORNL neutron sources, as described in Section 3.1.1. The key technical strengths of the unsurpassed peak brightness of cold neutrons, large bandwidth, and small beams will deliver the following science strengths, as described in the First Experiments report [4]:

- Time-resolved measurements of kinetic processes and beyond-equilibrium matter, real materials in operando
- Simultaneous measurements of hierarchical architectures from the atomic scale to the micron and beyond—multi-scale phenomena
- Measuring small samples of newly discovered or synthesized materials
- Special environments for exploring new frontiers in materials at extreme conditions.

The following items are within the project scope:

- Accelerator systems to transport protons from the existing SNS Ring-to-Target-Beam-Transport to the new STS target. The two SNS target stations will be able to run independently of one another.
- Target systems will provide a solid, rotating water-cooled tungsten target and two high-brightness coupled cold parahydrogen moderators.
- Instrument systems will construct 8 world-class neutron instruments and a bunker, which is a near-target monolith integrated shielding solution, that will support the eventual build-out of the remaining neutron beamlines.
- Conventional facilities will construct new buildings to house and support the new facility, including a target building and 40, 50, and 90 m instrument halls.
- Integrated controls will provide all control systems and computing infrastructure and the data acquisition systems for the neutron instruments.

Figure 3.1-2 illustrates the location and geometry of the STS and associated experimental halls. The project received Critical Decision (CD)–1 approval in November 2020 and entered the engineering/design phase.

Figure 3.1-2. Rendering of the SNS site after construction of the Second Target Station. STS buildings are shown in grey.

Second Target Station Initial Instrument Suite

A process to select the eight instruments constructed by the STS Project was launched in August 2020 with a call for proposals. Teams formed around 12 instrument concepts that had been discussed at previous user workshops. A committee of 22 national and international experts reviewed the proposals and provided rankings that guided the STS Project and NScD management selection of instruments to be built. In the words of the review committee, “The main finding of the committee is that all of the 12 instruments proposed are exceptionally strong, and they are all appropriate to be built at STS and would leverage the source characteristics to provide world-class scientific capabilities.” The eight instruments are listed, and Figure 3.1-3 illustrates early concepts.

- BWAVES—broadband spectrometer
- CENTAUR—small- and wide-angle neutron scattering instrument
- CHESS—cold neutron spectrometer
- CUPI^{2}D—neutron imaging
- EXPANSE—wide-angle NSE
- PIONEER—single-crystal diffractometer
- QIKR—kinetics reflectometer
- VERDI—polarized diffractometer

Two additional instruments will enter preliminary engineering design to provide options if funding permits their inclusion in the project or if the R&D efforts of one of the eight selected instruments is unsuccessful to a degree that precludes its construction: the TITAN extreme environments multimodal instrument and the M-STAR focused, polarized reflectometer.

Figure 3.1-3. Early concepts for the eight initial instruments to be constructed at STS.

The instrument proposal teams form the core of the instrument advisory teams that will remain engaged with the project throughout its lifetime. Instrument advisory team members will be invited to key design reviews, science decisions, workshops, eventual planning for sample environment equipment, and planning for commissioning and early science. The STS Project plans for continued engagement with the research community via instrument advisory teams, webinars and presentations by STS instrument scientists at national meetings, and workshops to develop a roadmap for building instruments on the remaining STS beamlines. Close coordination continues between the STS project and the operational SNS and HFIR facilities to ensure compatibility of the evolving hardware and software across the facilities. STS and its instrument suite are intended to be operated within a single organization, which also operates the SNS FTS and HFIR.

3.1.4 The HFIR Beryllium Reflector and Pressure Vessel Replacements

In addition to the SNS FTS PPU Project and the STS Project described (Sections 3.1.2 and 3.1.3), two major efforts are needed to meet the three-source strategy (Section 3.1.1) to provide neutron scattering capabilities optimized at three complementary and world-leading facilities. These efforts are the HBRR and the PVR.

HBRR is a necessary maintenance activity to replace the beryllium reflector and associated components due to radiation damage. It takes place roughly every 20 years. As part of the next HBRR, currently scheduled to start in 2028, the HFIR beam tubes and the cold source (HB-4 moderator vessel) will also be replaced. The associated interruption of routine reactor operations presents a rare opportunity to refurbish the network of cold neutron guides and to perform various upgrades of the scattering instruments in the guide hall and the beam room. Planning of this work has started with the goal of setting instruments up for world-class operation and performance for the next 20 years. Figure 3.1-4 shows the current model of the future instrument landscape in the HFIR cold neutron guide hall, which includes a guide hall expansion as well as new and relocated instruments.

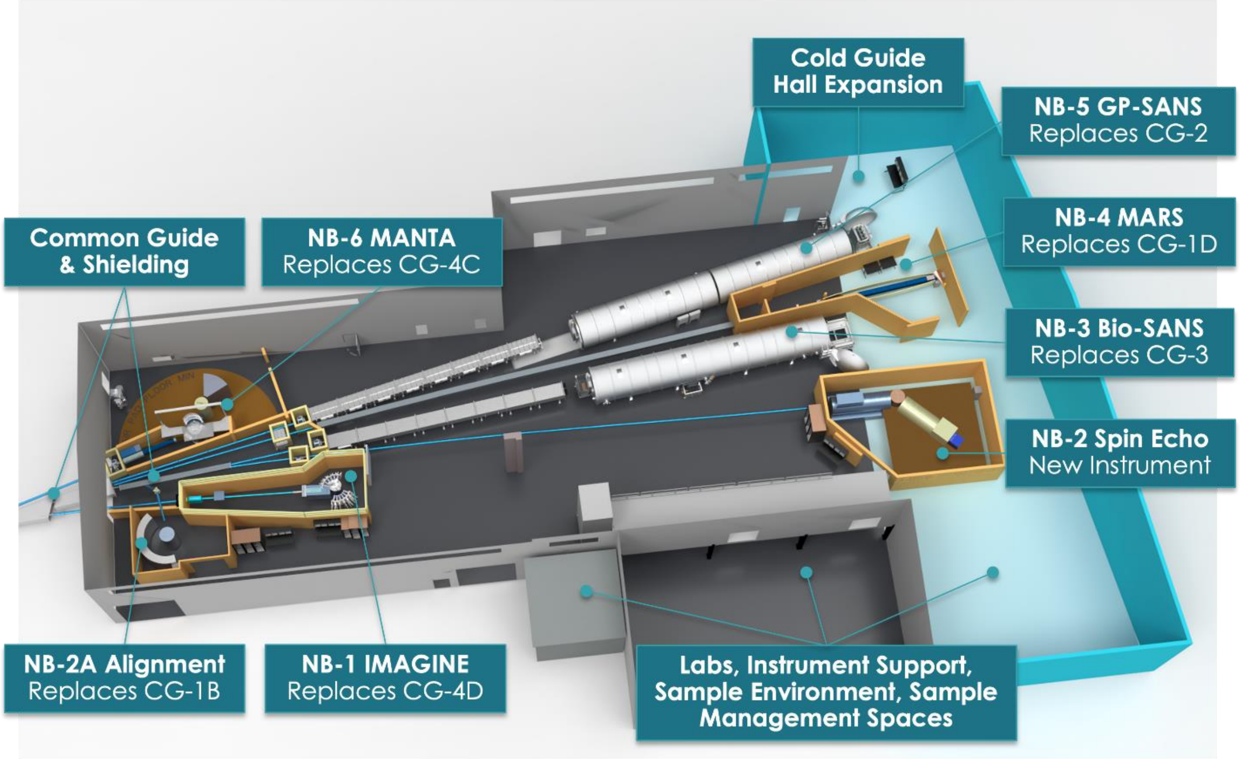


Figure 3.1-4. Current model of the future instrument landscape in the HFIR cold neutron guide hall.

The HFIR PVR project was initiated in response to a recent BESAC subcommittee which was convened to assess the scientific justification for a US domestic high-performance reactor-based research facility. One of its key recommendations was to replace the HFIR pressure vessel to extend its life for another 50 years or more [2]. The PVR is a multiyear project to evaluate and implement upgrades to the pressure vessel and associated reactor components that will allow future enhancement of the scientific capabilities of all HFIR stakeholder programs at ORNL (Neutron Sciences, Physics, Isotope Science, Fusion, and Fission Science) that could be made possible by the PVR. The current plan is to execute the project in two phases with phase 1 covering the design, procurement and assembly, and phase 2 the installation, with an expected gap between the two phases of several years. The vessel components would be installed and aligned in the new vessel, which will be kept in the new Fabrication, Assembly, and Materials (FAM) building for long term storage and mitigate against unexpected, accelerated degradation of the existing pressure vessel.

As part of this effort, studies for commensurate capability enhancements in neutron scattering began in 2021. A new pressure vessel will enable beam tubes (HB-2 and HB-4) with an enlarged diameter, and a new beryllium reflector assembly will allow a change of direction for these tubes (Figure 3.1-5). The two most significant outcomes from such changes for neutron scattering will be (1) the possibility to lead a manifold of thermal beams into a new thermal guide hall downstream of HB-2 and (2) the capability to insert a neutron guide into the HB-4 beam tube to better guide the beams toward the center of the existing guide hall for much improved neutron transport.

Figure 3.1-5. Concept of modified beam extraction at HB-2 and HB-4.

Constructing a new second guide hall on the HFIR site was another key recommendation of the BESAC subcommittee report [2]. A concept for a new thermal neutron guide hall is shown in Figure 3.1-6. This facility will offer several transformative advantages over the present configuration of the thermal instruments. These instruments are currently located in the beam room, close to the reactor core. This arrangement leads to two challenges at HFIR that significantly limit the thermal neutron scattering capabilities: (1) the beam room has a very small spatial footprint and no large overhead crane access, limiting the size and number of instruments that can be installed, and (2) the high neutron background greatly degrades the signal-to-noise performance of those instruments.

This investment in a new thermal neutron guide hall will pay off with a far superior, new level of capability for serving the research needs of the nation in the areas of quantum materials, energy, chemistry, materials science, engineering, and soft matter. Distancing the thermal neutron instruments from the source greatly reduces the background and simultaneously expands the space available for additional instruments without negatively affecting the neutron beam flux. This results in greatly improved signal-to-noise enabling measurements from smaller samples and detection of weaker signals, which are typically associated with, for example, inelastic features, superlattice peaks, or magnetic scattering. The addition of the thermal guide hall will be further leveraged by more widespread implementation of polarized neutrons and polarization analysis.

Moving most of the thermal instruments out of the beam room also eliminates potential reactor safety concerns, enabling the use of high-power magnetic fields, high-pressure gas systems, and other extreme environments. Furthermore, a new thermal guide hall will provide expanded laboratory and development space allowing these ancillary capabilities to be located near the beamlines. Overall, this setup will attract a much broader user base that currently cannot be served.

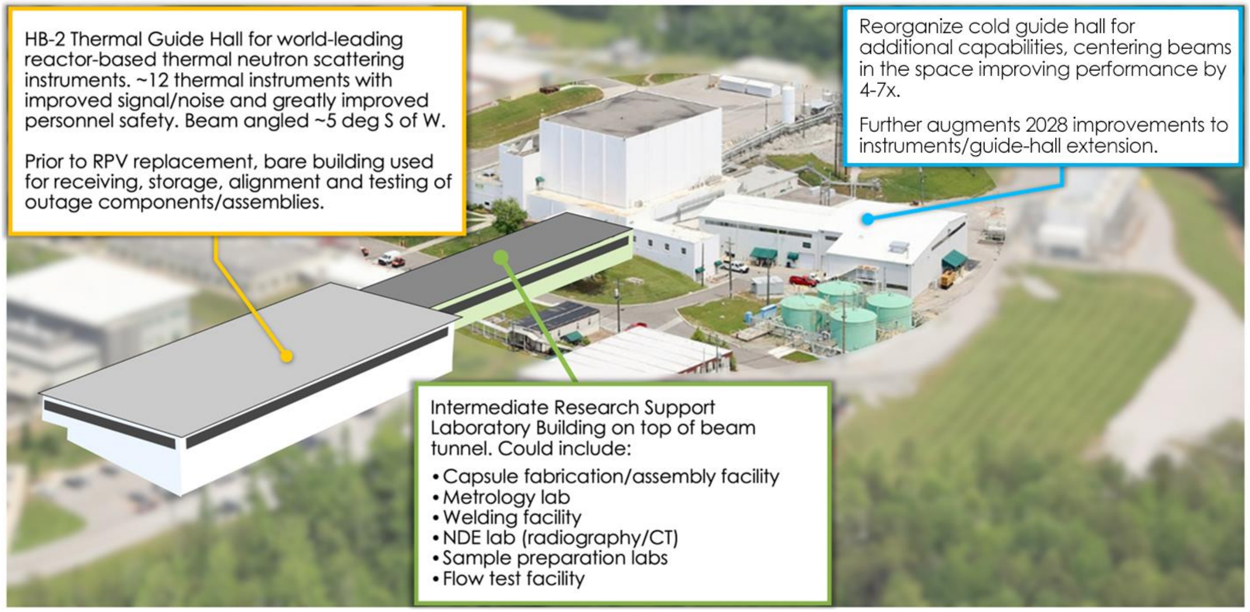


Figure 3.1-6. Concept of new thermal guide hall building.

A renewed suite of thermal scattering instruments at HFIR in a new thermal guide hall will be developed. It could include:

- A polarized single crystal diffractometer
- A high-flux powder diffractometer
- A high-resolution powder diffractometer
- A strain scanning diffractometer
- A polarized triple-axis spectrometer
- An unpolarized high-flux triple-axis spectrometer
- A chopper spectrometer
- Other future concepts.

3.2 Instrument Suites

Section 3.1.1 describes our vision for a three-source strategy that will ensure that our scientific user community will have the best neutron scattering capabilities to meet the scientific challenges of the future. In this section, we describe our vision for the neutron scattering instrumentation for the next 10 years. We describe our current suite of instruments at HFIR and SNS, and our process for continuously updating and upgrading them to keep them current and competitive to ensure that we continue to meet the user community's expectations. We then describe our vision for new instrumentation, which is strongly based on the recommendations of the 2018 ORNL Neutron Sciences Instrument Advisory Board [5] and on a continuous evaluation of the needs of the five strategic science areas described in Section 2. The Instrument Advisory Board report recommended the construction of four new instruments (VENUS and DISCOVER at SNS, and MANTA and an NSE instrument at HFIR). As scientific priorities and technological capabilities evolve, there will be a need to build additional instruments in the future. A new process has been initiated for selecting and prioritizing additional instruments at FTS, STS, and HFIR that will evaluate the science needs and use a holistic approach that optimizes the placement of all instruments across the three sources to maximize their overall neutron scattering capabilities and scientific impact.

3.2.1 Instrument Suites at HFIR and SNS

Neutron beam instruments at ORNL include a wide range of techniques broadly characterized as diffraction, small-angle scattering, reflectometry, radiography (imaging), and spectroscopy. Of the 30 instruments, 18 are located at SNS (Figure 3.2-1), and 12 are located at HFIR (Figure 3.2-2).

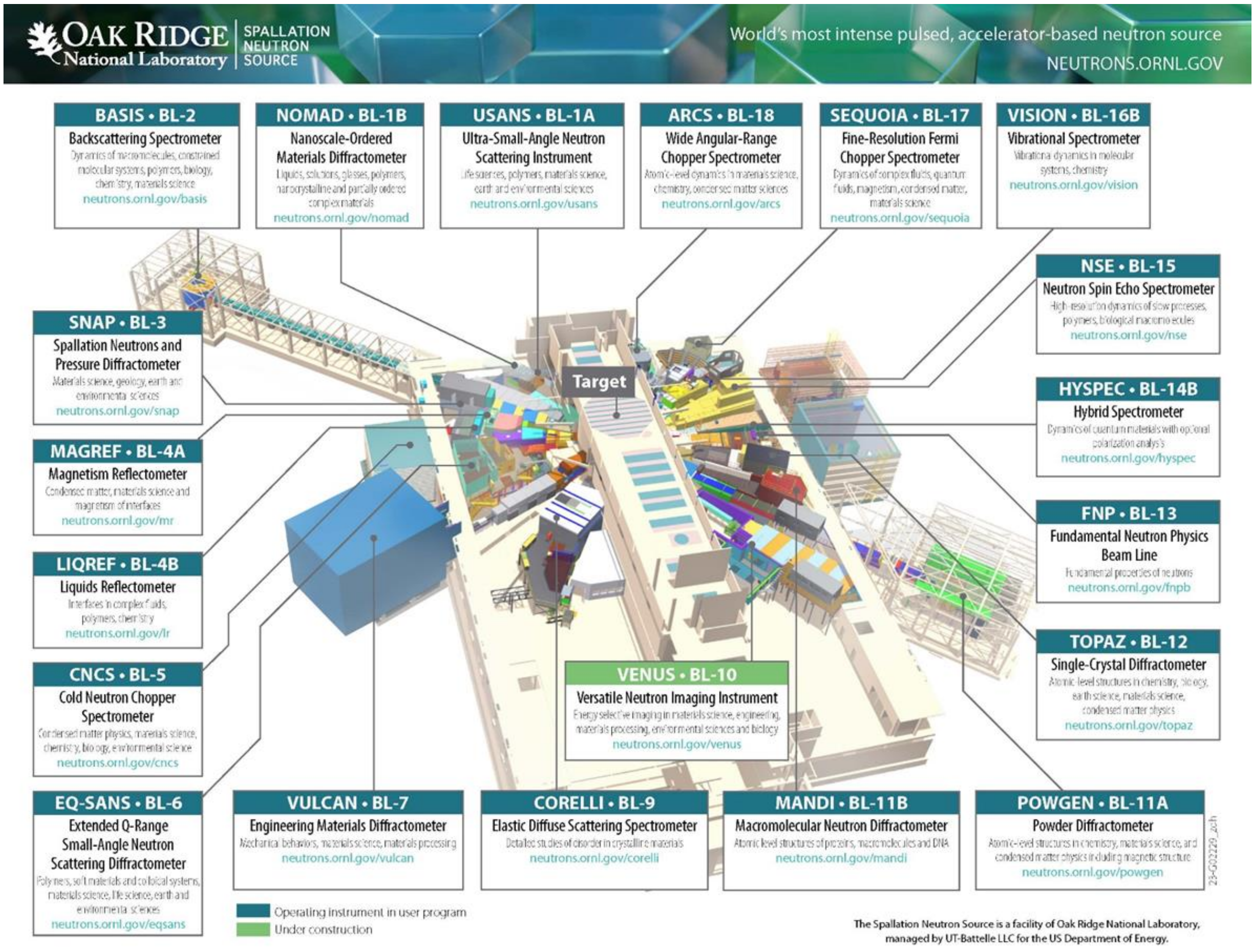


Figure 3.2-1. Layout of neutron beam instruments at SNS. This layout includes 18 neutron instruments in the neutron scattering program, 1 fundamental physics instrument (Section 4.2.3), and 1 instrument under construction (VENUS [BL-10]).

The diffraction instruments can be grouped into single crystal diffractometers, powder diffractometers, and specialized instruments with a focus on materials engineering. For single crystals, the SNS suite consists of CORELLI (BL-9, diffuse scattering), and two wavelength resolved Laue diffractometers MANDI (BL-11B, for macromolecular materials) and TOPAZ (BL-12, high-resolution diffraction). At HFIR, the suite consists of DEMAND (HB-3A, four circle or 2-axis modes) and IMAGINE (CG-4D, Laue diffractometer for biological studies). Powder diffraction instruments at SNS include NOMAD (BL-1B, high flux) and POWGEN (BL-11A, high resolution). At HFIR, the suite consists of POWDER (HB-2A) and WAND^2 (HB-2C, using a high-resolution 2D detector). Specialized instruments include VULCAN (BL-7, engineering components and materials in situ, operando, and under mechanical loading) at SNS and HIDRA (HB-2B, residual stress analysis) at HFIR for engineering diffraction, as well as SNS's SNAP (BL-3, high-flux, medium-resolution instrument) emphasizing studies under extremes of pressure and temperature.

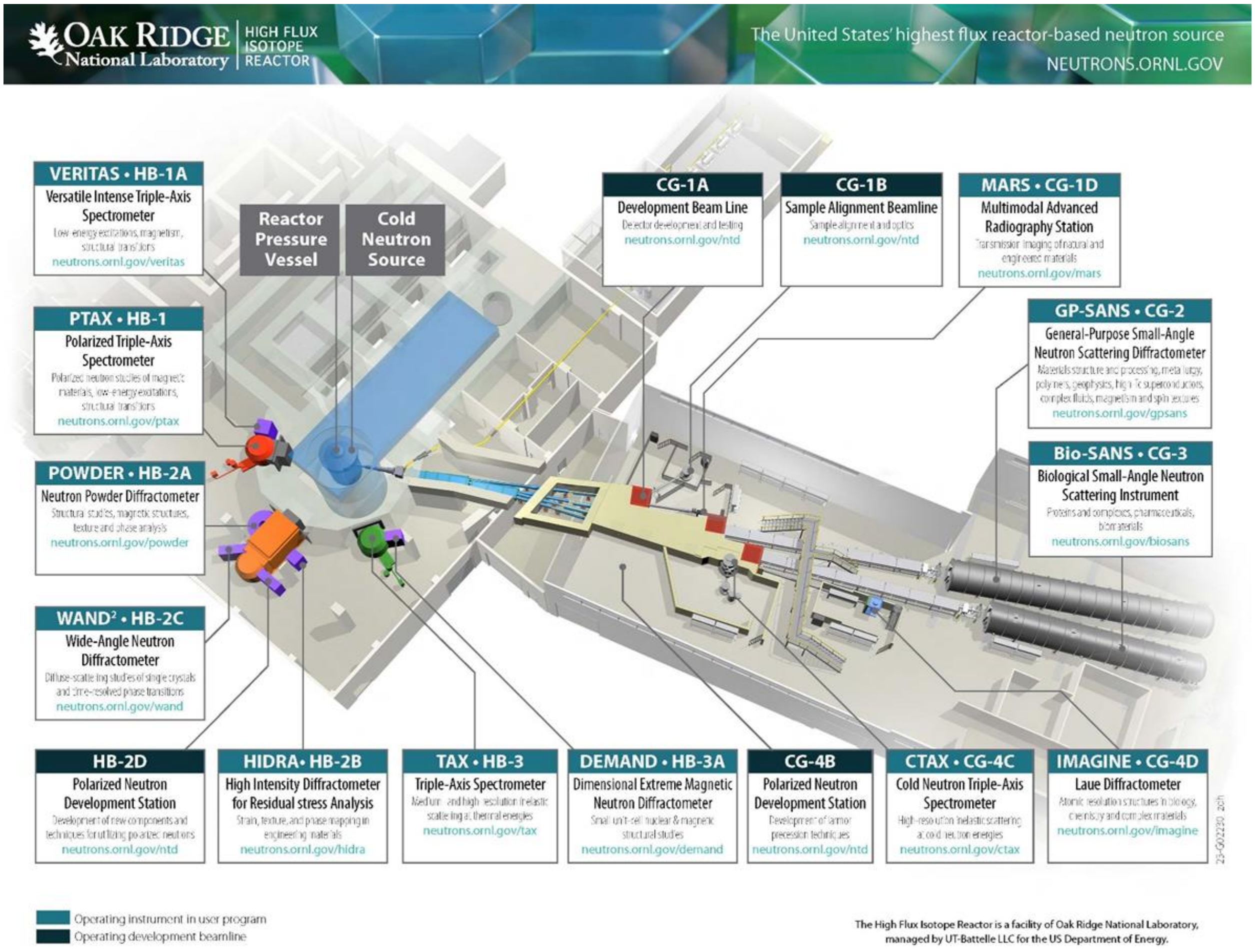


Figure 3.2-2. Layout of neutron beam instruments at HFIR. This layout includes 12 neutron instruments in the neutron scattering program, 2 development instruments, and a sample alignment station.

The SANS instruments include GP-SANS (CG-2), BIO-SANS (CG-3) and EQ-SANS (BL-6). GP-SANS and BIO-SANS are nearly twins and have many identical components. They are standard pinhole SANS instruments with velocity selectors for selecting a bandwidth of neutrons from the HFIR cold source. GP-SANS has the highest neutron flux, and, as the longest of the three SANS instruments, resolves the lowest momentum transfer $Q_{\mathrm{min}} = 0.0007$ Å^{-1}. BIO-SANS features two spatially separated detector banks, providing the widest angular coverage and a dynamic range $Q_{\mathrm{min}}/Q_{\mathrm{max}}$ of up to 300 in a single measurement. EQ-SANS is a TOF wavelength-resolved pinhole SANS instrument. It can attain the highest maximum Q of the three SANS instruments. Thanks to wavelength-resolved TOF data, it also provides finer resolution at high angles, making it especially useful for applications in well-ordered periodic structures, such as in membrane diffraction. The USANS instrument (BL-1A) at SNS is a Bonse–Hart double-crystal diffractometer. The fine angular resolution of the double-crystal diffractometer's optics resolves lowest values of $Q = 1 \times 10^{-5}$ Å^{-1}: the Q-range of the USANS overlaps with and greatly extends beyond the maximum size of structural features that are measurable on the other three SANS instruments. The reflectometers are the MAGREF (BL-4A,) and LIQREF (BL-4B) at SNS. MAGREF employs beam geometry with reflection from a vertical sample plane and uses polarized neutrons, making is suitable for distinguishing between magnetic and nuclear scattering from the sample. LIQREF has a beam geometry with a horizontal sample surface, enabling studies of liquid (fluid) interfaces, which are especially important for studies of soft matter and biological samples such as lipid membranes. Neutron radiography and tomography studies are conducted at the HFIR MARS (formerly

IMAGING; CG-1D) instrument as well as on a fraction of the beam time at SNS SNAP (BL-3). A new TOF wavelength-resolved imaging beamline, VENUS (BL-10), is presently under construction at SNS.

The spectroscopy instruments are grouped into triple-axis spectrometers, direct-geometry spectrometers, and spectrometers for molecular spectroscopy. HFIR has four triple-axis spectrometers. VERITAS (formerly FIE-TAX; HB-1A), PTAX (HB-1), and TAX (HB-3) are thermal triple-axis instruments. VERITAS is a fixed-incident energy instrument, PTAX is a polarized triple-axis spectrometer using polarizing Heusler monochromator and analyzer crystals, and TAX is a versatile instrument with three monochromator crystals that can be selected by computer control. HFIR has one cold triple-axis spectrometer, CTAX (CG-4C). The direct-geometry instrument suite at SNS consists of two instruments on decoupled water moderators, SEQUOIA (BL-17) and ARCS (BL-18), and two instruments on coupled cold moderators, CNCS (BL-5) and HYSPEC (BL-14B). SEQUOIA is optimized for higher resolution measurements with a longer flight path, and ARCS is optimized for wider angular coverage. CNCS is a high-resolution cold neutron direct-geometry spectrometer, and HYSPEC is optimized for polarization analysis measurements using a Heusler crystal to polarize the incident beam and a supermirror array to analyze the scattered neutrons. The molecular spectroscopy suite is composed of two indirect-geometry spectrometers, VISION (BL-16B) and BASIS (BL-2), together with one NSE instrument, NSE (BL-15). VISION selects its final energy using pyrolytic graphite analyzer crystals enabling vibrational spectroscopy for energy transfers up to approximately 600 meV. BASIS is a near-backscattering geometry indirect-geometry spectrometer that uses silicon crystals to select the final energy to enable quasi-elastic measurements. NSE is a TOF NSE spectrometer that uses the Larmor precession of neutrons in a symmetric pair of magnetic fields (encoding and decoding zone before and after the sample) for ultrahigh resolution of very small energy transfers, which are characteristic, for example, in the slow dynamics of soft condensed matter.

3.2.2 The Center for Structural and Molecular Biology: a DOE Biological and Environmental Research–Funded Collaboration

The Center for Structural Molecular Biology (CSMB) is a DOE SC BER–supported structural biology resource. The CSMB supports the scientific and user program of the BIO-SANS (CG-3) instrument at HFIR. BIO-SANS is dedicated to the analysis of the structure, function, and dynamics of complex biological systems. This program also operates SNS's Bio-Deuteration Laboratory, which supports production of a variety of deuterated biomacromolecules and biologically relevant small molecules for the SNS/HFIR biology user program. This resource complements capabilities at other DOE SC BER facilities for structural biology and supports studies of biomass recalcitrance and biomembranes as part of the DOE SC BER Genomic Science Program. BIO-SANS science topics include biomacromolecules and assemblies, biomembranes, and hierarchical structures with a particular emphasis on studies of lignocellulosic biomass for biofuels and bioproducts.

To broaden the impact of the CSMB and catalyze the synergy between DOE SC BER–funded structural biology resources, we established a collaborative program with the National Synchrotron Light Source II for joint access to SANS and small-angle x-ray scattering (SAXS) and the DOE BER Facilities Integrating Collaborations for User Science (FICUS) initiative between the Joint Genome Institute (Lawrence Berkeley National Laboratory), the Environmental Molecular Sciences Laboratory (Pacific Northwest National Laboratory), and the Advanced Photon Source (Argonne National Laboratory).

3.2.3 Instrument Upgrades, Science Productivity Program

Maintaining and upgrading NScD's neutron scattering instrumentation to current standards is essential to ensuring the ability to serve the user community and to meet future science challenges and national needs. The first SNS neutron scattering instruments are already 15 years old, and some of HFIR's instruments are more than 20 years old. The NScD Science Productivity program provides a systematic process to identify and prioritize major instrument improvements and upgrades that are aligned with NScD's strategic planning. This program is managed by a Science Productivity Steering Committee, comprising senior scientists and managers, that conducts rolling reviews and assessments of instrument capabilities and major instrument improvement projects and provides directorate-level recommendations on instrument priorities, impacts, and resource allocation. The Science Productivity Steering Committee (1) identifies major instrument projects, (2) sets instrument priorities and resource allocation, and (3) executes and manages projects/resultant actions.

The instrument assessments are ongoing and holistic, and instrument improvement projects are prioritized to address opportunities for major instrument developments, such as increased detector coverage, beam polarization components, collimation, sample environment, and software needs. The instrument assessments are supplemented with the recommendations from instrument suite beamline review panels. These external panels review the mission need, technical capabilities, scientific impact, and productivity, as well as planned upgrades of all the HFIR and SNS instruments on a triennial basis.

The science productivity process continues to evolve as new opportunities, scientific needs, and community needs are identified. In addition to identifying instrument improvement projects, the process will be expanded to guide the future development and construction of new instruments at HFIR and SNS. This guidance would apply to new instruments beyond the instruments recommended in the 2018 the Instrument Advisory Board report (VENUS and DISCOVER at SNS, MANTA and NSE at HFIR) described in Section 3.2.3 and to new instruments at the STS beyond the STS Initial Instrument Suite (Section 3.1.3). This new process would involve an external advisory committee composed of researchers from outside of ORNL, and an internal expert committee, both of which would be appointed by the NScD Associate Laboratory Director. The internal expert committee would evaluate concepts and proposals for new instruments in their early stages, while the external advisory committee would review the full proposals and make recommendations to the associate laboratory director about which new instruments should be built.

3.2.4 New Instruments

3.2.4.1 VENUS, the VErsatile Neutron imaging InstrUment at SNS

A world-class neutron imaging instrument—VENUS (VErsatile Neutron Imaging InstrUment at the Spallation Neutron Source; BL-10)—is being built to uniquely utilize the SNS intrinsic TOF capabilities to measure and characterize large-size and complex systems. VENUS is optimized to measure microscale structures by using both radiography (2D) and computed tomography (3D). VENUS enables a broad range of science, including energy materials, materials science and engineering, biology, and geosciences. The beam is optimized for TOF imaging techniques (i.e., Bragg edge and resonance imaging). These novel TOF imaging techniques complement HFIR's existing MARS (CG-1D) beamline at HFIR, which currently serves the General User Program and is optimized for attenuation-based microscopy. Although VENUS is designed to provide the largest field of view of all imaging beamlines and is optimized to operate across a broad range of neutron energies, from epithermal to cold, the future STS CUPI^{2}D imaging beamline will exclusively use cold neutrons for fast kinetics and characterization over the broadest time and length scales, using techniques such as TOF neutron grating interferometry and Bragg edge imaging. This capability is achievable because STS will increase the cold neutron flux by a factor of 40 compared with FTS.

The VENUS user community comprises academia, industry, and government laboratories. VENUS will provide the opportunity to advance scientific research and enable new scientific discoveries in the areas of advanced manufacturing methods such as additive manufacturing, functional materials, transportation, engineering, industrial technologies, geosciences, plant physiology, and biology. VENUS can help answer basic research questions. The in situ characterization of new electrical energy storage materials will contribute to increased battery efficiency and storage density, spanning from the atomic (using Bragg edge imaging) to mesoscopic (with attenuation-based or conventional imaging) scales (Section 2.4.3, "Batteries/Energy Storage"). Investigating the behavior of superalloys will elucidate the mechanical behavior of advanced manufacturing components during stress (Section 2.3.1, "Transformative Manufacturing"). Resonance imaging will enable investigation of advanced nuclear materials in extreme environments (Section 2.3.2, "Materials for Complex Reactor Environments"). VENUS can also contribute to the understanding of the processes associated with complex and heterogeneous subsurface mineral assemblages that comprise porous rock formations and the complex fluids flow residing across several time and length scales. This understanding will shed light on the natural soil carbon reservoir (Section 2.4.2, "Carbon Cycle, Carbon Dioxide Capture, Conversion, and Storage").

VENUS is currently under construction with an anticipated early completion date of June 2024. The overall layout of the VENUS beamline is illustrated in Figure 3.2-3. The beamline includes three main sections: (1) the front-end optics, (2) the instrument cave, and (3) the radiological materials area and control hutch. The beamline is designed to provide the following unique capabilities:

- Bragg edge imaging (cold and thermal neutrons) with a wavelength resolution ($\Delta\lambda/\lambda \approx 0.20\%$) in the thermal and cold range to map Bragg edges in a crystalline structure to assess microstructure properties such as crystalline plane orientation, grain orientation, and/or strain with a maximum field of view of 20 cm × 20 cm.
- Resonance imaging (epithermal neutrons at energies from approximately 1 eV to a few hundred electron volts) with a maximum field of view of 4 cm × 4 cm at a spatial resolution of 150 µm (or better as detector technology improves)

VENUS will also have the capability to (1) provide conventional attenuation-based contrast (white beam [i.e., or a wide wavelength spectrum over several angstroms]) radiography and computed tomography and (2) investigate large regions of interest using thermal/cold neutron white beam at a spatial resolution of approximately 50 μm with a region of interest of approximately 20 cm × 20 cm.

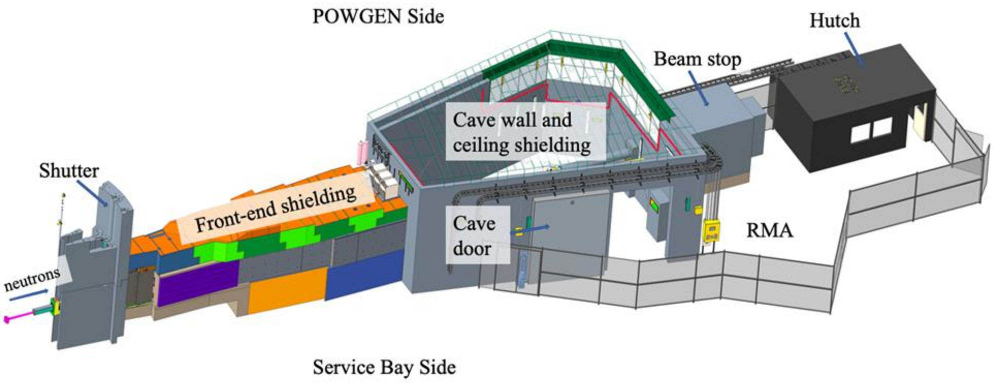


Figure 3.2-3. General layout of the VENUS instrument (BL-10). Pictured are the shutter, front-end optics, cave walls and ceiling, cave door, beam stop, radiological materials area, and control hutch.

3.2.4.2 DISCOVER, a Total Scattering Neutron Diffractometer for Materials Research

DISCOVER, a new instrument proposed for the SNS FTS, will help drive the US economy with a critical role in expanding the creation and improvement of materials and structures that affect people's daily lives. The discovery of new materials has played an enabling role in all aspects of modern civilization, ushering in new energy, security, health, and information technologies. The DISCOVER beamline will deliver new functionality, supplying the scientific community with a total neutron scattering platform for frontline investigations of the delicate interplay of global and local atomic symmetries, for examining how order evolves from the atomic to the macro scale, and for discovering how these features respond to external perturbation. Key scientific opportunities include the following fundamental studies of chemical and physical materials processes:

- Expanding the possible materials and structures that can be made (as described in Sections 2.3.1 and 2.3.2)
- Uncovering design rules for new energy storage technologies (such as those highlighted in Section 2.4.3)
- Advancing reactive material interfaces for chemical separations, conversion, and utilization (as described in Sections 2.4.1 and 2.4.2)
- Ushering in new paradigms for controlling emergent states of quantum matter (by providing the structural information, at a local, medium, and long-range scale, Sections 2.1.1 and 2.1.2)
- Deploying modern computational/analysis tools for unprecedented rapid discovery cycles

DISCOVER will both require and fully exploit the characteristics of FTS at SNS and therefore will be highly complementary to existing and future powder diffractometers at STS and HFIR. Currently, FTS has two powder diffractometers, NOMAD (BL-1B; the Nanoscale Ordered Materials Diffractometer) and POWGEN (BL-11A; the General-Purpose Diffractometer). NOMAD is a high-flux, low-to-medium resolution diffractometer, and POWGEN is a low-to-medium flux, medium-to-high resolution diffractometer. Both are used for detailed structural studies of a wide range of materials. NOMAD and POWGEN are highly complementary: they are at opposite ends of the flux vs. resolution trade-off. However, critical scientific questions in materials discovery cannot be answered without combining the needed resolution, *Q*-range, and flux metrics in a single instrument. DISCOVER will provide not only this capability but also the two critical aspects of enhanced physical access and low scattering backgrounds at the sample position.

As a result of its in situ and operando coupled diffraction and pair distribution function mission, the DISCOVER instrument must deliver a high *Q*-space resolution along with a sufficiently wide wavelength band to cover a broad range of *Q*-space in a single instrument measurement. A rendered end-to-end engineering design of the DISCOVER concept is pictured in Figure 3.2-4. The instrument will be situated at beam port 8B at the high-resolution side of the ambient temperature water moderator at SNS. It will deliver a wavelength band of 1.6 Å (3.2 Å in a two-frame mode). A focusing guide designed to optimally illuminate a sample area of 8 mm × 10 mm will be used; however, the instrument will be able to accommodate larger samples (up to 25 mm tall) to increase scattering intensity at reduced resolution. DISCOVER will use position-sensitive ^{3}He tubes as detectors, arranged along a logarithmic spiral around the sample position. The instrument will be compatible with the current TOF diffraction sample environment suite as well as an elevating sample platform, providing access to modular user-based sample environments. A comprehensive preconceptual design estimates that this essential instrument could be delivered to the user community in 5 years once funding has been allocated.

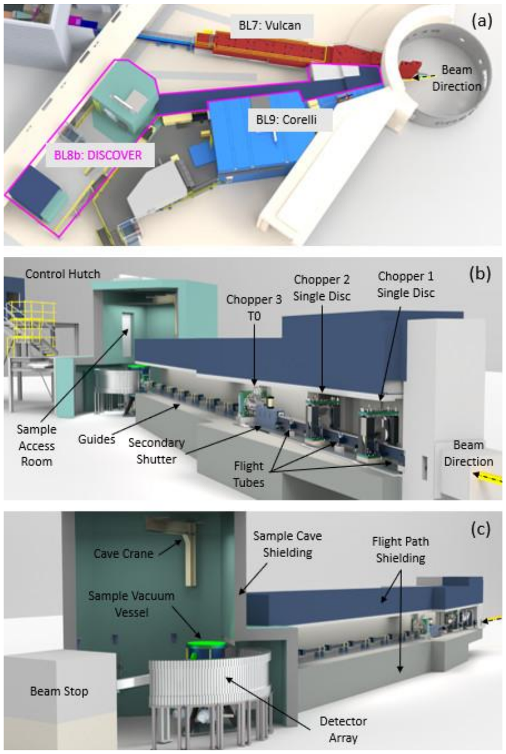


Figure 3.2-4. Rendered end-to-end engineering design of the DISCOVER concept. (a) DISCOVER will be located on BL-8B at SNS, between VULCAN (BL-7) and CORELLI (BL-9). The design leaves space and incorporates shielding to accommodate a future BL-8A instrument between DISCOVER and VULCAN. (b) DISCOVER viewed toward the sample access room and control hutch. Several optical components of the beamline are labeled. (c) DISCOVER viewed upstream, toward the source. Several major instrument cave and shielding components are labeled. In (b) and (c) the shielding has been removed from the near side of the beamline to display internal instrument components.

3.2.4.3 MANTA, Multi-Analyzer Neutron Triple-Axis Spectrometer

The proposed Multi-Analyzer Neutron Triple-Axis (MANTA) instrument will provide critically needed world-leading capabilities for cold neutron spectroscopy to the quantum materials community. As a world-class cold triple-axis spectrometer at HFIR, MANTA will facilitate unique low-energy neutron spectroscopy experimental capabilities that are in high demand by the quantum materials community. The high flux of continuous neutrons provided by MANTA will enable crucial parametric studies as well as polarization tensor measurements to be undertaken that are currently difficult or impossible. MANTA, combined with the cold neutron TOF spectrometer CNCS (BL-5) at SNS and the next generation spectroscopy capabilities of CHESS at STS (Section 3.1.3), will provide the unprecedented complementary capabilities to the US quantum materials community required for the United States to retain a position of leadership in this emerging research area. Using a modified CTAX (CG-4C) back end will allow for polarized neutron scattering experiments to accompany polarization capabilities at HYSPEC (BL-14B) and PTAX (HB-1), including the use of Wollaston prisms and Larmor techniques.

Because the instrument will provide the capability to measure novel quantum phenomena, the core user community for the proposed MANTA instrument will be users measuring quantum materials. The challenge of classifying the static and dynamic correlations in spin liquid candidates is a growing area for quantum information (Section 2.1.1). Cold neutron instruments have proven invaluable in this effort, and the flexibility of MANTA to measure under a range of conditions with polarized neutrons would provide new opportunities for measuring topological and spin liquid materials. The large increase in cold neutron flux from the re-optimized front end of MANTA will enable new scientific capabilities, particularly in the measurement of small samples, interfaces, and thin films, which will create opportunities to measure novel quantum materials and discover new quantum states. Neutrons are well suited to measuring quasiparticle lifetimes (Section 2.1.2) of such phases to characterize the quantum fluctuations that drive these phases.

The MANTA spectrometer is a proposed cold neutron spectroscopy instrument for the NB-6 position in a re-optimized cold guide hall at HFIR. The initial phase of the project involves building a new primary spectrometer and relocating the back end of the CTAX spectrometer at the NB-6 position in a re-optimized cold guide hall. The NB-6 position on the new cold neutron guide will be better suited to a triple-axis instrument because it will view the cold source more directly, leading to a higher neutron flux on the monochromator. The redesign of the guide system will also allow for the inclusion of a velocity selector and an incident beam v-cavity polarizer. The neutron velocity selector will be used to eliminate higher order neutron wavelengths, which will reduce the background and spurious features in the measurements. The v-cavity will be placed on a translation stage to allow for the quick transition between unpolarized and polarized modes, enabling new science to be conducted that is not currently possible on CTAX.

The CTAX back end will be modified to accommodate the beam profile of MANTA and to provide polarization analysis capabilities through a removable v-cavity. It will also be designed to allow for use of Wollaston prisms and Larmor techniques, complementing these capabilities on the thermal triple-axis spectrometer (TAX [HB-3]) at HFIR. MANTA will see significant gains in flux compared with the CTAX spectrometer as a result of its large view of the cold source, modern guide design, and double-focusing monochromator that will ensure it is competitive with other world-class cold triple-axis spectrometers around the world. Simulations of the front-end optics indicate that MANTA’s flux will be approximately 50 times higher than the current CTAX spectrometer. These flux gains are significant for conventional triple-axis experiments and are of the order needed to enable polarization analysis, the use of pressure cells, and inelastic measurements of small samples. These capabilities will dramatically increase the science that can be performed at HFIR and will position MANTA as a world-class cold triple-axis instrument.

Phase II of this instrument will involve construction of a multiplexed back end (Figure 3.2-5). The multi-analyzer and multi-detector configuration will use a vertical scattering geometry with multiple analyzer crystals stacked along the scattered beam to provide quasi-continuous coverage over the instrument’s *Q*- and *E*-range. This spectrometer will increase the phase space that can be measured, particularly for inelastic measurements that cover a wide *Q*- or *E*-range. This back-end upgrade will be built to retain the capability for polarization analysis, making it a complementary instrument to the suite of spectrometers at HFIR and SNS. The single analyzer and multiplexed back-end options will be interchangeable, depending on the scientific requirements of the individual experiments, increasing the scientific impact of the MANTA instrument.

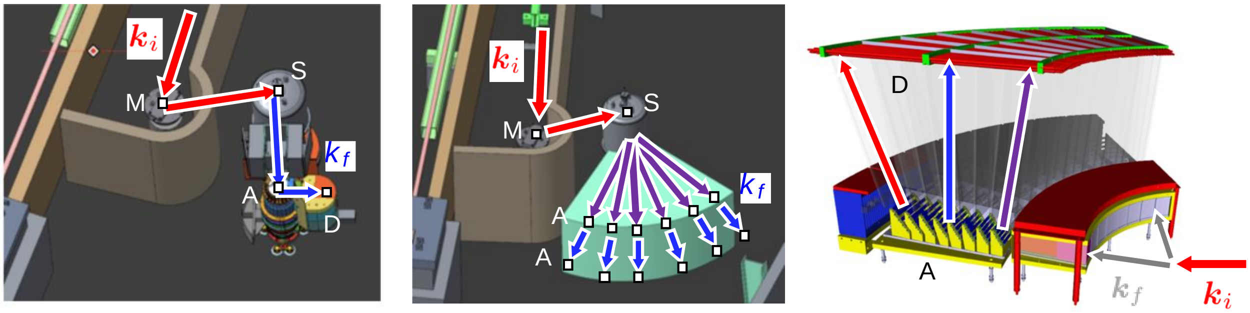


Figure 3.2-5. Overview of the MANTA Project. (a) Phase I: Relocation of the modified CTAX (CG-4C) secondary spectrometer to a new fully optimized end-guide location. (b) Phase II: Implementation of a multiplexed secondary spectrometer. (c) Schematic of the secondary spectrometer for the CAMEA instrument at PSI.

3.2.4.4 HFIR Neutron Spin Echo

Among neutron scattering techniques, neutron spin echo (NSE) spectroscopy is unique in measuring slow relaxation dynamics. The construction of a high-resolution monochromatic NSE spectrometer at HFIR will enable world-leading research in the field of polarized neutron spectroscopy by providing a unique combination of high-energy resolution and large dynamic range. The high-flux high-resolution HFIR-NSE will be a world-class instrument that will address the user community science requirements (e.g., the use of revolutionary small-size samples to make the technique accessible to major biomedical applications). HFIR-NSE will provide the high neutron intensity, stability, and reproducibility required by many of the relevant macromolecular systems that exhibit low concentrations of the mobile species but very high background from the matrix material (e.g., per-deuterated polymers, nanocomposites, complex fluids, and colloids) and will cover a broad *Q*-range and large Fourier time values.

By combining a modern design of fringe field compensated solenoids with optimized field shape coils that can guarantee high intrinsic field integral homogeneity without the need for strong corrections, the HFIR-NSE spectrometer could reach Fourier times of hundreds of nanoseconds at a particularly low field integral, corresponding to short-to-intermediate wavelengths (8 Å ≤ λ ≤ 10 Å) for which the scattering intensity is particularly high, enabling a dramatically reduced measurement time. This capability will address the longtime requests from the biological and medical scientific community for the investigation of biomacromolecules, drug design, and drug delivery systems with reduced lifetime, as well enable in situ observation of relaxation processes. Also, the availability of longer wavelengths in the HFIR beam spectrum will expand even further the dynamical resolution of the HFIR-NSE spectrometer.

The NScD long-term vision is that the HFIR-NSE will replace SNS-NSE (BL-15) and will complement the wide-angle spin echo spectrometer EXPANSE at STS (Section 3.1.3). These two spectrometers will complement each other in the energy resolution and dynamical range, offering the user community an unprecedented combination of quasi-elastic dynamics techniques.

The HFIR-NSE spectrometer will address mostly the strategic science areas of biological materials and systems (Section 2.5) and soft matter and polymers (Section 2.2). It will provide new views on soft condensed matter research directed toward mesoscopic time and length scales, predominantly in the small-to-intermediate angle *Q*-range regime and very large Fourier times in the order of hundreds of nanoseconds (100 ns ≤ HFIR-NSE Fourier time ≤ 700 ns). HFIR-NSE likely will also be useful to probe the local dynamics of quantum materials (Section 2.1) and other systems in which long-range order is not always present. Complementary to HFIR-NSE, the EXPANSE spectrometer at STS will operate well within the very high scattering angle regime, up to 3.5 $Å^{-1}$, featuring a very short Fourier time range (30 ps ≤ EXPANSE Fourier time ≤ 10 ns), addressing the user community from strategic science areas such as quantum materials, chemistry, and engineering.

The HFIR-NSE spectrometer will be optimized for small sample volumes. The spectrometer will be situated on the NB-2 beamline and will take full advantage of its positioning at HFIR to achieve the following capabilities:

- The highest flux intensity at long wavelength (i.e., large Fourier times)
- The highest flux intensity at medium-to-high Q-range among all NSE spectrometers
- The lowest possible intrinsic field integral inhomogeneity
- The best available correction elements
- The shortest counting time per sample among all NSE spectrometers
- The best stability and reliability over long counting times
- The possibility of a threefold reduction in the sample volume

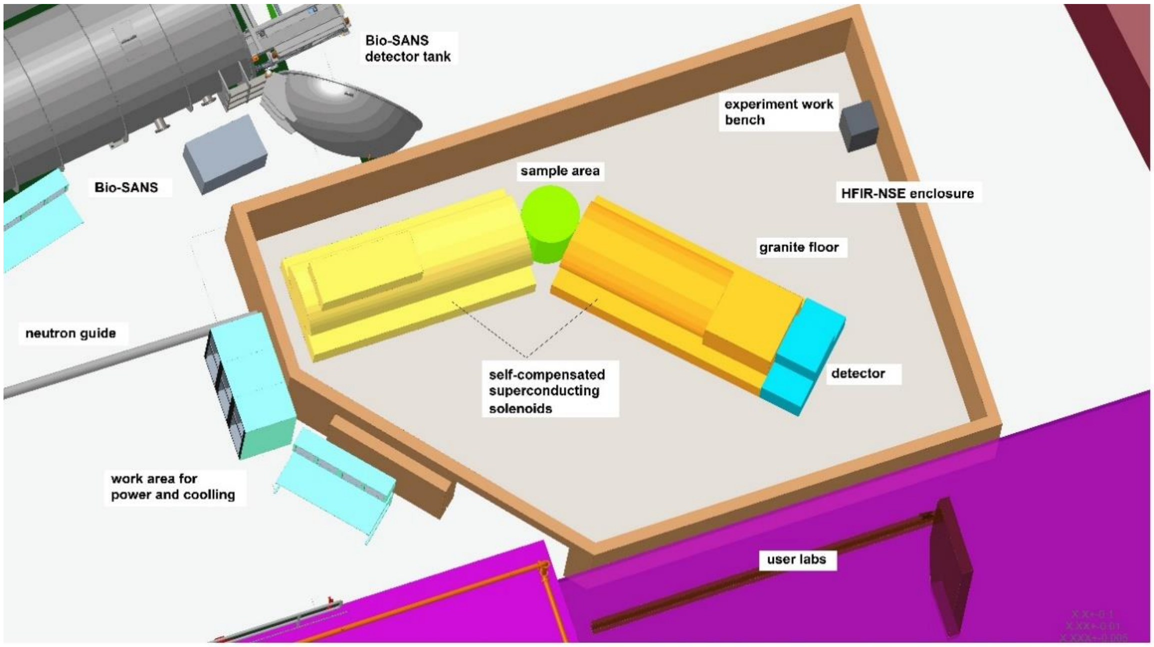


Figure 3.2-6. The envisioned HFIR-NSE design and its situation in the HFIR cold guide hall. Two superconducting solenoids, the sample stage, and the detector are shown. The brown enclosure represents the spectrometer shielded area around the granite floor. ,

The requirements for a new NSE spectrometer in the cold guide hall at HFIR are an integral part of the HBRR development project. The overall layout of the envisioned HFIR-NSE in the HFIR cold-neutron guide hall is shown in Figure 3.2-6. The main NSE components (e.g., the self-compensated superconducting magnets) require custom design and manufacture and a production-to-delivery time that can range between 3 and 5 years. The extension of the HFIR guide hall, the construction of a non-vibration nonmagnetic granite floor for HFIR-NSE, the design and installation of a new guide system to deliver high flux at long wavelength at the sample-area position, and securing the necessary project funds place the construction into a 10 year planning window.

3.3 Instrumentation Control, Data Acquisition, Reduction, and Analysis

Scientific computing plays an essential role in the delivery of high-impact research outputs from neutron scattering investigations. Providing visiting researchers with access to state-of-the-art scientific computing infrastructure and functional and performant software systems and data services increases the rate at which high-quality neutron data can be analyzed, interpreted, and published.

The 10 year vision for ORNL NScD scientific computing builds upon a firm world-leading position in the area with the following ambitious but achievable objectives that together benefit the entire science program across the whole instrument suite:

- Ensure that that all users leave SNS and HFIR with reduced and corrected data sets and at least an initial data analysis that can be refined after their visit in collaboration with facility staff and their research group. Applying the concept of data analysis as a service will provide a far more efficient research workflow. Improve the accessibility to neutron science for experienced and inexperienced user communities by providing support to perform data analysis and data interpretation.
- Enable new experimental modalities with next-generation data acquisition systems and instrument control, leveraging new technologies such as ML and AI to provide automation and autonomous control. For example, kinetic time-resolved experiments such as those described in Section 2.4.3 where SANS data can be acquired and processed in real time to map functional processes in battery charging that can be augmented with simple classification algorithms to allow intelligent mapping of phase space.
- Develop and implement investigation-specific data management plans to allow users to efficiently manage their data and access data services from central computing infrastructure. Build on the current use of industry-standard data and metadata management to provide integration opportunities with sister facilities and domains, allowing ML/AI technologies to be robustly and repeatably deployed. ML/AI methods are increasingly used in NScD’s domain to augment mission-critical data services. Development of standards for management of training data sets and models will become as important as traditional management of raw experimental data.
- Enable real-time or near real-time data processing, visualization, and analysis, thereby providing the capability to efficiently use neutron beam time. This capability relies upon high-performance data pipelines that in turn can be integrated with HPC-based modeling and simulation. Such systems are routinely used for chemical spectroscopy and provide insight into, for example, catalysis functionality and lattice dynamics of functional materials such as metal organic frameworks.
- Build sustainable collaborations for data services with the user community and stakeholders to provide a key element of codesign of data methods to deliver improved user experience and functionality. Building collaborations between user facilities and between user facilities and HPC centers will enable enhanced levels of data integration within the research infrastructure community, with the objective that user communities will benefit from the capability of dataset co-analysis and improved accessibility to complex modelling and simulation methods.
- Provide the user community with open-source, performant, and trusted software systems for data reduction and data analysis that include corrections for complex scattering phenomena. Coupling such capability with Monte Carlo beam transport simulations and calculation of scattering cross sections provides the framework to develop digital twins of beamlines and samples.

Sections 2.1 through 2.5 demonstrate the unique scientific advances that modern neutron scattering science affords the scientific community from environmental science to quantum materials. Specific core infrastructure development, including advances in data acquisition technology and data processing, provide a firm foundation for all science program areas. Development of data pipelines and data workflows enable real-time data analysis and increased application of ML/AI methods to accelerate the analysis and interpretation of neutron data.

Future data analysis standards will include increased access to HPC infrastructure, ab initio codes, and molecular dynamics simulation software results that are effectively used as experimental digital twins. This data analysis modality builds upon current standards for molecular spectroscopy and inelastic scattering. Extending these workflows to other experimental modalities provides improved insight into the material properties required for high-impact research outputs.

Providing users with access to complex data services that add value to the experimental research is essential for research infrastructures. For example, digital models of the dynamics and microscopic interactions of molecules and crystalline surfaces in mesoporous media are essential to interpret data from neutron investigations of carbon sequestration and gas separation. HPC environments and state-of-the-art atomistic simulation facilitate investigation of interactions between viruses and small molecules. Developing accessibility to such data services should include providing visiting researchers with access to data interpretation that is agnostic to their previous experience. In so doing, research infrastructures can deliver services to a far broader user community and fully exploit the experimentally measured quantitative neutron cross sections.

The development of the ORNL instrument suite with new instruments and detector upgrades (Sections 3.2 and 3.5) together with upgrades to neutron sources (Section 0) provide users with unique experimental capability, delivering higher data rates and increased experimental throughput. Capability development within the area of scientific computing provides facility users with the correct tools to manage and interpret neutron data. For a paradigm in which the data volume and velocity of data acquisition increases, user communities will develop research programs across the research infrastructure environment, the use of ML/AI methods will become routine, and integrated data pipelines and workflows then become an essential architecture. Thus, to meet the need of more than 1,000 annual investigations with gigabyte/terabyte datasets, integrated data pipelines and workflows are an underlying component to success.

The development of the functionality in scientific computing for the existing facilities and instruments should dovetail with the anticipated needs and requirements of the STS project, which itself provides new challenges for this area.

The achievability of this strategy leverages several key factors including building upon existing interdivision and interdirectorate collaborations. Thus, ensuring the neutron user program benefits from the breadth and depth of the on-site expertise in all areas of the data chain, from data acquisition to delivery of HPC. These broad crosscutting collaborations, founded on best practice open-source research software engineering methods, provide the agility needed to deliver performant systems and enable collaborations with sister facilities and communities.

Specific details of NScD’s key objectives are discussed in Sections 3.3.1 through 3.3.4.

3.3.1 Instrument Control and Data Acquisition

The primary needs of the instrument control and data acquisition systems for the next decade can be summarized in the following three core capacities:

- Capability to handle neutron flux rates of at least two orders of magnitude higher than 2020 levels
- Capability to handle the corresponding increase in raw data storage

- Capability to enable real-time data reduction, analysis, and visualization that incorporates new technologies using ML and AI

As detailed in Figure 3.5-1 in Section 3.5, the science need for detector performance with rates of 5×10^9 counts/s is targeted for availability by 2030. Section 2 refers to the need for ML to be incorporated into feedback loops within the instrument control system, underscoring the need for real-time data reduction as well as the need for significant computational resources to be placed at the beamline. Only after data reduction can decisions be made about what part of the sample or what change to the environment is needed for the next probe of the sample.

The SNS and HFIR data acquisition software uses a set of software components collectively named Accelerating Data Acquisition, Reduction, and Analysis (ADARA). A collaborative project between SNS and ORNL's Computing and Computational Sciences Directorate [6], ADARA provides a real-time publish/subscribe network streaming data acquisition system that gives researchers nearly instant access to their experimental data both during and after data collection.

Figure 3.3-1 shows the computing system components that are operational for users in 2022 (achieving a sustained rate of 1.5×10^7 counts/s, with corresponding raw storage requirements, but limited real-time reduction or analysis). Note that the distributed nature of the architecture lends itself very well to participating in multifacility shared resources. The remainder of this section describes the plan for updating these components to be able to sustain these rates and enable the real-time reduction and analysis capabilities described in Sections 3.3.2 and 3.3.3.

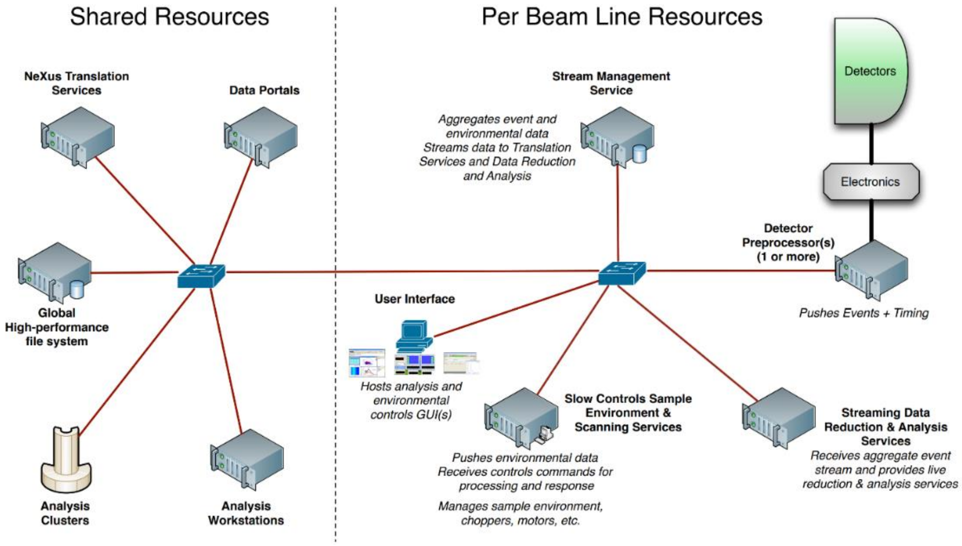


Figure 3.3-1. Streaming data analysis and acquisition infrastructure, as operational in 2022. Red lines indicate high-performance network connections that enable the neutron instrument data stream to multiple client systems.

3.3.1.1 ADARA Next Generation

To achieve the needed increase in neutron event throughput, upgrades must incorporate advances in heterogeneous computing that are occurring in the commercial sector. These systems fuse computing and networking together such that more functions are performed by the network: data can be transformed in transit, which saves time because the data undergoes fewer passes through storage systems.

First, ADARA will update its key component, the streaming-message-server (SMS). The update will add the capability of the SMS to execute on these programmable network devices. Joining the SMS to the optimized storage and network infrastructure is the evolution needed to scale up to the 5×10^9 event rate throughput. Second, the streaming-translation-client component of ADARA will be enhanced to provide the diverse formats required for the data reduction systems, as detailed in Section 3.3.2. Finally, ADARA will update its implementation of the streaming data reduction and analysis services. Advances in compiler technology have progressed to the point that algorithms described in one system (Mantid) may be recast into another system. Therefore, scientists will use the analysis workstations to define the needed algorithms and then schedule them to be used for live reduction by an automated process. This process will ensure that the specified algorithm is error free and suitably performant on the requested computational resource.

3.3.1.2 Storage, Networking, and Computing Infrastructure Upgrades

To achieve the 5×10^9 event rate, the networking infrastructure at each beamline must be updated to 200 G speeds (the product of 5×10^9 and 32 bits/event is 160 Gb/s). This speed is possible because the current state-of-the-art networking speed in cloud data centers is currently 400 Gb/s, as is the ESnet, a collaborative science network connecting national laboratories and academic institutions [7]. By 2030, 100 Gb/s networking is expected to be as ubiquitous as 10 Gb/s networking is in 2022.

The detector preprocessor and the stream management service are combined into one machine. Electronics with high-rate networking adapters are added to allow several detector assemblies to combine into one readout point for the ADARA stream, collocated with the beamline storage. The storage in the stream management service expands to contain the capacity to hold unreduced event data from approximately 1 week of operation.

Direct connection from the stream management service to the streaming data reduction and analysis service is made using high-rate networking. The streaming data reduction and analysis computer is enhanced with electronics to execute ML codes that can operate the software described in Section 3.3.3 together with the live reduction code. This computer becomes the source of the feedback control that allows ML to drive the instrument to new positions as directed by these algorithms. Furthermore, it enables streaming to other systems for immediate visualization.

The goal of the storage, networking, and computing upgrades is to enable real-time visualization of the experiment progress directly in the scientific domain in conjunction with the model the users use to understand the behavior of the sample they study. Achieving this goal requires close cooperation with the data reduction and data analysis to operate in a compatible machine execution environment. The data reduction and analysis, the user’s simulation models, and the visualization of these results require the combined effort of all three groups to achieve this goal.

3.3.2 Data Reduction

Neutron scattering users are currently able to reduce and process their data for the existing instrument suite. However, during the next 10 years, techniques employed by the instruments will continue to evolve, the instruments themselves will evolve (e.g., changes to detector configuration, additional sample environment), new instruments will be built, software technologies will evolve, and correction techniques will evolve. Recent efforts to modernize existing software are expected to continue.

The goal of data reduction at the end of the next 10 years is to provide reduced files in formats for preferred applications, from a web interface, that are available in near real time. These goals will enable in situ measurements for which users can view the reduced data throughout the experiment to aid in decision-making. This capability requires technological improvements as well as changes to how experiments are performed. The experiment team, consisting of ORNL staff and visiting researchers, will need to inform the system of how the data will be measured. In exchange, the system will need to be prepared to re-reduce when the measurement does not go as planned.

3.3.2.1 Metadata Capturing

Capturing metadata, the data that describes the raw data is an essential requirement of NScD’s data management strategy to provide findable, accessible, interoperable, and reusable (FAIR) data.

A considerable of amount of metadata can be autonomously scraped from the control system, as is routine, and saved into standardized hierarchical data format version 5 containers using the NeXus data format. The more challenging form of metadata is that which provides provenance and context to the dataset. Current practice is to store these data in logbooks either on instruments or by the visiting scientists. The objective is to develop investigation-specific data management plans that describe key provenance metadata and provide a convenient method of ingestion into the experimental dataset. This can then be archivally persisted with a digital object identifier (DOI) for use in publication submissions.

Beyond the ambition to make data FAIR, metadata is essential for automation systems that operate on data steams or as part of automated data-processing workflows.

To reduce and process raw data, the software must be informed of all the parameters needed to process it. By providing the information as early as possible, the data can be reduced as soon as it is available. All the information is known at some point, but often the user prefers to measure samples before backgrounds or needs some extra information or experience with the experiment to decide binning parameters or reciprocal space cuts. The flexible nature of the experimental workflow provides a certain challenge for automated systems that rely upon digital information from the control system or on the existence of preexisting data files.

Whenever possible, process information will be gathered by connecting to operating systems rather than requesting the information a second time (from the user). Information decided at experiment configuration time (e.g., what run files to combine) will be passed from the data acquisition system. Information that is provided by the instrument team (e.g., appropriate calibration) will be confirmed by the local contact and generated early for the running experiment to ensure that measured data are still useful even if an unexpected outage stops the experiment early.

Some metadata are derived as part of the experimental process (such as orientation matrix information) These derived parameters can be passed to the data acquisition software for use in subsequent measurements.

3.3.2.2 Streaming Data

The STS is expected to have very high data rates. Even at the FTS, VENUS (BL-10) (under construction) and NOMAD (BL-1B) (recently upgraded) have data rates that are a challenge to traditional data reduction approaches. Currently, data are reduced once the NeXus file is made available, and the process of reading the data to process it is an unnecessary bottleneck. Similar to the major work done within the data acquisition system, the data must be reduced while they are being measured to aid in situ measurements and reduce the time it takes before users see data in a form they can easily understand. Processing streaming data will better inform users how their experiments are progressing, so they have more time to think and adjust their measurement strategy.

Currently, live-data reduction produces images for the monitoring site (monitor.sns.gov), but its use is limited, and little effort has gone into verifying whether the live-reduced data are identical to the data reduced from NeXus files. The validation and verification step is critical. Additionally, a clear data retention policy will be determined and communicated. Intermediate results to be reviewed must be stored, at least temporarily, but these results can have a significantly shorter lifespan than those that are published in journals. Published reduced data will be associated with digital object identifiers, or DOIs, to allow them to be referenced in the associated publication. Depending on how fast a portion of the data reduction workflow takes, it may be more appropriate to always calculate certain results on demand rather than store them.

3.3.2.3 Reduction of In Situ Measurements

Event-based data reduction was a defining feature of SNS from its early design stages. For sparse data, it provides improved performance, smaller memory footprint, and reduced artifacts from (effectively) smoothing the data. More recently, event-based data reduction has been used for filtering the data based on an ancillary environment that varies slowly (>1 s). This process has proven difficult when creating many slices. Already, instruments are looking toward in situ measurements and slicing within a proton pulse. Expanding event-based data reduction to support this mode of operation will allow for measurements of chemical reactions, battery charge/discharge cycles, gas capture/release cycles, and much more. Significant effort must be spent to engineer a solution that is more performant, increases the total number of slices that can be made available, and accounts for the sample environment when the neutron was scattered rather than when the neutron was detected. Also, the formalism for determining the sample condition when the neutron is being scattered will be determined.

3.3.2.4 Fostering the Open-Source Software Community

Scientific computing at HFIR and SNS is a longtime proponent of free/libre open-source software (FLOSS) and open data standards. As evidenced by NScD's long term involvement in the NeXus data standard and the Mantid project collaboration. By fostering FLOSS and open data standards, the facilities have given experimenters greater access to their raw data, as well as the capability to inspect how the data were processed. HFIR and SNS intend to continue to grow their footprint with strategic participation in scientific software projects, either by contributing to or joining existing projects, or by creating new projects that in which the scientific community is encouraged to participate.

The objective is to develop all scientific software under an appropriate open-source license, making it freely available for use by the scientific community.

3.3.3 Data Analysis

Data analysis enables extraction of scientific knowledge from neutron data and, as such, represents a key component in the neutron data pipeline. Advanced neutron instrumentation, producing unprecedented volumes of data, and problems of increasing complexity often cause data analysis, modeling, and simulation to be a bottleneck in scientific output and impact from NScD's neutron sources. Furthermore, coupling with advanced theory is often needed to generate the most influential publications. As such, a strategy for data analysis is critical to broadly enable science across the user community. Continued success is based on a comprehensive assessment of current and future needs across instrument suites and scientific communities and close collaborations across ORNL, between scattering facilities, and with experts in the user community.

Data analysis at a user facility can be broadly divided into two categories: standard analysis and advanced analysis. Here, standard analysis comprises the steps that are needed to extract a scientific result for a standard experiment on a given instrument. Advanced analysis includes analyzing data from nonstandard experiments, requiring advanced materials modeling and/or theory. Clearly, the latter requires the most significant development and can benefit significantly from close interaction between NScD's Neutron Scattering Division and the Computer Science and Mathematics Division. A previous proof-of-principle project jointly developed between the Neutron Scattering Division and the Computer Science and Mathematics Division, the Integrated Computational Environment for Modeling and Analysis (ICEMAN), demonstrated the potential of employing scientific workflows in the interpretation of neutron data. An opportunity exists to build on the ICEMAN work and develop a general platform for neutron data analysis, modeling, and simulation. A 3 year focused Laboratory Directed Research and Development initiative, the *Neutron Data Interpretation Platform Ecosystem*, began in FY 2022. This initiative will be composed of a series of projects, including advancing the platform together with projects to develop a series of applications for advanced data analysis and modeling.

3.3.3.1 Real-Time Data Analysis

The need for real-time analysis is growing. This area will concentrate on developing analysis tools and workflows to enable computer-guided or automated experiments, which will require consideration of the entire experiment workflow from acquisition to reduction to analysis. Projects in this area will greatly benefit from collaboration across ORNL to leverage their development efforts. Current priorities are the following:

- Real-time data analysis tools to study solid-state reactions in situ and make decisions on the fly (*Catalysis of green ammonia for H storage*)
- Rapid computed tomography reconstruction for MARS (CG-1D) (*multiple areas*)
- Real-time data analysis methods to obtain 3D reconstruction of morphologies under different operating conditions (*High-performance energy storage systems*)
- Rapid multimodal data analysis and acquisition incorporating external parameters such as temperature fields (infrared) and distortions (digital image cross correlation) and other control parameters (e.g., power, deposition speed) (*Transformative manufacturing*)

3.3.3.2 High-Performance Computing Materials Modeling

One of the unique strengths of neutron scattering is that the nuclear and magnetic cross sections can be readily calculated, allowing a quantitative comparison to theoretical models and calculations. Although computationally intensive modeling techniques can be used to compare neutron data, this effort tends to be expert based. Modular workflows can be developed to reduce the barrier to such advanced modeling approaches and can enable production of synthetic data from methods such as DFT, molecular dynamics (MD), quantum Monte Carlo (QMC), density matrix renormalization group (DMRG), and dynamical mean field theory (DMFT). The OCLIMAX software contained within ICEMAN converts DFT results into simulated data, enabling virtual neutron spectroscopy experiments to be performed. This conversion is a form of digital twinning, and the approach taken in OCLIMAX can be implemented across different instrument types and areas of science. Current priorities are the following:

- For catalysis, use DFT as well as AI-based tools like DeepMD to simulate very large systems (Catalysis of green ammonia for H storage)
- For protein dynamics, calculate vibrational and relaxational dynamics over many orders of magnitude (DFT, MD, ab initio MD) (Biocatalysis)
- For crystallography, use quantum mechanics/molecular mechanics methods with DFT approaches to correctly describe metal centers (Biocatalysis)
- Obtain access to simulations such as QMC, DMRG, DMFT (Quantum materials for quantum information)

- Construct data analysis workflows harnessing the power of virtual experiments including utilization of computing resources outside ORNL (Quantum materials for quantum information)
- Conduct advanced simulations of soft matter including DFT, MD, and coarse grain simulations (High-performance energy storage systems)
- Use materials simulation models to simulate macro-mechanical/micro-mechanical (crystal plasticity), thermal (heat transfer), and chemical (phase field) response for prediction of additive manufacturing materials properties (*Transformative manufacturing*)

3.3.3.3 Artificial Intelligence/Machine Learning Applications

Broad community interest in ML methods has led to several studies that explore the potential use of such approaches in neutron scattering. ML has demonstrated the potential for feature identification, background and artifact suppression, and materials property prediction and classification. Despite this potential, R&D is needed to develop and deploy ML workflows for automated or streamlined interpretation of neutron data. Current priorities are the following:

- Use AI-based tools like DeepMD to simulate very large systems (*Catalysis of green ammonia for H storage*)
- Employ AI/ML methods to identify the appropriate analysis method for SANS/reflectometry (*Biocatalysis*)
- Combine data and state-of-the-art theory by applying AI/ML and large-scale modeling to enable close integration of theory and experiment (*Quantum materials for quantum information*)
- Train surrogates to quickly analyze and simulate experiment choices (*Quantum materials for quantum information*)
- Use AI/ML methods that can streamline data interpretation to incorporate large-scale simulations (*High-performance energy storage systems*)

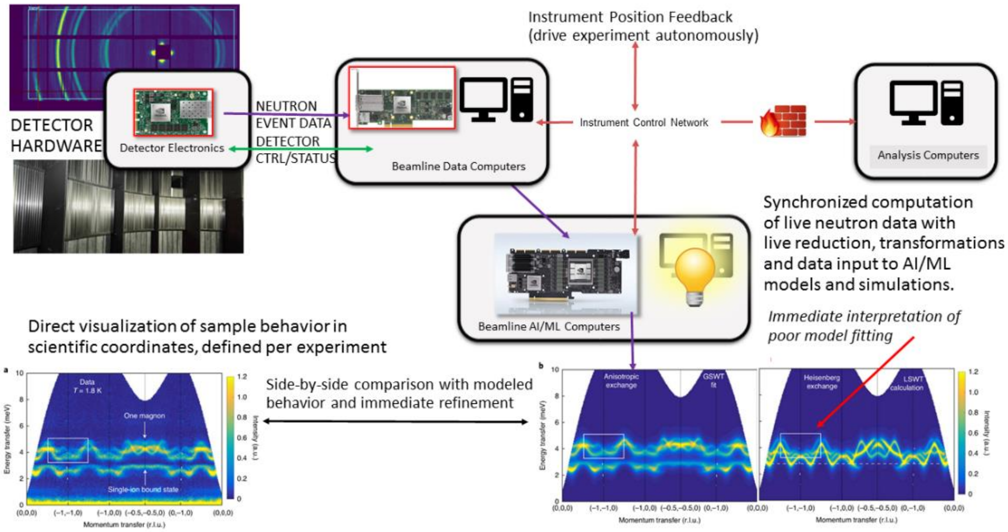
3.3.4 AI/ML Driven Experiment Control and Automation

The updates described in Section 3.3.1.2 will allow the facility to take advantage of the next frontier in instrument control: experiment automation beyond sample alignment and into directed search. Neural networks (NNs) provide approximate solutions to problems that are described by probability gradients. NNs enable unsolvable problems to become solvable under certain conditions. The NN produces the solution’s parameters and, with the necessary augmentation, can detect when the conditions are such that those parameters are invalid. The act of incorporating NNs into a software process is ML, and systems that use ML in their compositions are AI. Using the right NN incorporated into a feedback mode with the instrument control is the difference between a search based on human intuition and experience (and unconscious bias) and a data-driven search. Scientists program the NN, and then the NN can operate over vast amounts of data—orders of magnitude more than the scientists could process on their own. Using AI/ML leverages the computational power of very large scale integrated electronic circuits and the characteristics of NNs to become a force-multiplying tool for the scientist.

Projects are already underway at SNS and HFIR to incorporate ML to identify and optimize multi-axis sample alignment of crystallography experiments [8], to analyze and determine optimal tomographic projections [9], and to incorporate optical feedback control over sample positioning [10]. Although instruments routinely use conventional (non-AI/ML) feedback systems based on deterministic computations of (slowly varying) control system data, the experiments at POWDER (HB-2A), SNAP (BL-3), TOPAZ (BL-12), and VULCAN (BL-7) are pioneering the needed software interfaces for AI/ML feedback control of experiments.

To illustrate the science-enabling aspects of AI/ML feedback control and automation, three topical areas are provided in this report as examples. The development of design rules for biomembranes needed for neuromorphic computing, as discussed in Section 2.5.2, involves using hydrogen/deuterium isotopic labeling and neutron reflectometry to probe the in-plane structure of candidate membranes. By collecting data under a variety of environmental conditions, an NN can help explore the design space of these membranes to assist in determining the optimal topological structure of these biomolecules. The validation of simulation theory through experimental measurement, as discussed in Section 2.5.1, uses computational feedback between experimental data acquisition, reduction, and analysis systems and quantum simulations of the parameters of entanglement, state, and coherence.

Figure 3.3-2 illustrates this process; for example, the analysis of an experiment performed on the SEQUOIA instrument (BL-17) required weeks of computing and scientist time. Incorporating AI/ML infrastructure into the instrument data acquisition system offers the possibility to perform the visualization and parameter refinements as the experimental data are collected. AI/ML processes can also enable new science by completing the coupling of neutron scattering with multiphysics models, as discussed in Section 2.3.1: transformative manufacturing. Feedback control in operando experiments can provide the sought-after understanding by implementing fast-surrogate models and adaptive control in every experiment that allows refinement and validation of the models' parameters. Such coupling is not trivial, and success requires a concerted effort in software and computational engineering to achieve a response to deriving model parameters at an appropriate timescale.



Xiaojian Bai, Et. Al., "Hybridized quadrupolar excitations in the spin-anisotropic frustrated magnet FeI2", Nature Physics Letters 17, April 2021
https://neutrons.ornl.gov/content/neutrons-piece-together-40-year-puzzle-behind-iron-iodide%E2%80%99s-mysterious-magnetism

Figure 3.3-2. Diagram of an instrument control system that enables scientific visualization and live model refinement with AI/ML feedback control. (a) Experiment data transformed into scientific coordinate systems. (b) Simulations of modes with equivalent parameters.

The goal of AI/ML-driven experiment control and automation is to use the instrument's machinery to direct the neutron beam to the sample to cover the parameter space being searched. Only neutron event and fast metadata-driven ML can achieve this goal because the scattered neutrons hold the information needed to extract the atomic order, phase transition, and response to environmental conditions that the sample is undergoing. With the infrastructure enhancements proposed in Section 3.3.1.2, dedicated engineering collaborations, and the support of DOE, this goal is achievable.

3.4 Sample Environments, Sample Preparation, and Complementary Techniques

A successful neutron scattering experiment depends on the user's ability to precisely and accurately control experimental parameters such as temperature, pressure, and magnetic fields. Reliability means that the sample environment equipment performs to its required functions (e.g., controls temperature, pressure) under stated conditions (e.g., vacuum, inert atmosphere, magnetic field) for a specified time (e.g., experiment duration) in routine and/or unexpected circumstances. Sample environment development must be agile and responsive to the science needs, which are by nature diverse and rapidly evolving. State-of-the-art techniques and capabilities should be developed in the core areas of magnetics, low temperatures, high pressures, high temperatures, and soft-matter environments. Over the next 10 years, NScD will continue to automate the routine functions of the equipment so that more effort can be directed toward custom experiment setups. Environments will be developed to use a combination of laser light or microwaves with low temperatures and magnetic fields to probe nonequilibrium states of matter. Environments will be developed to use multimodal probes to investigate structural and thermodynamic properties over extended time and length scales. To achieve these scientific productivity goals, NScD's sample environment program must be world leading in both operations and development.

3.4.1 Sample Environments for Soft Matter

All scattering experiments use sample environments to apply/maintain the necessary physical or chemical conditions and/or to induce a sample into a state of interest. Therefore, they are an integral part of any proper scientific experiment and not accessories. However, going forward, neutron sample environments must also interrogate samples under conditions that are similar to those used by other physical measurements so that the scattering data can be used to provide complementary information. New and thoughtfully designed sample environments for soft matter will expand the users' research possibilities, thus making neutron scattering techniques more appealing to the general user and ever more relevant to 21st-century science. The following subsections outline such new sample environment developments.

3.4.1.1 Liquid Surfaces and Interfaces

The underlying principles for generating intelligent behavior in living organisms are fundamentally different from those used in traditional silicon-based circuits, in which memory and data processing are co-localized. Although different platforms are used to characterize the electrical properties of many neuromorphic systems and devices at the nanoscale, including their energy storage and dissipation properties, currently no practical experimental techniques can determine the structural features that are responsible for the nonlinear features of neuromorphic systems. With the appropriate liquid sample environments, neutron reflectometry offers the real possibility to understand how structural membranes reorganize memory and learning to biologically relevant neuromorphic systems. Neutron reflectometry sample environments with built-in electrical measurements and the capability to create relevant physicochemical conditions will produce data that inform the fabrication of robust soft-matter-based neuromorphic computation devices. They will also improve the ability to understand how memory and learning manifest in the human brain, opening new vistas in neuroscience, including the potential for novel approaches to treat devastating brain diseases and disorders.

3.4.1.2 Aligning Materials in Magnetic Fields

The amount of structural and dynamic information accessible from a neutron scattering experiment can be correlated to the sample's degree of orientation. For example, compared with powder samples, highly aligned membrane systems provide more robust structural information, including in-plane and out-of-plane structures. Moreover, data acquisition is accelerated, increasing sample throughput. However, the fabrication of highly aligned soft materials on solid supports (e.g., single crystal of Si) is nontrivial, and unwanted influences can be imparted to the sample from the substrate. However, some soft materials (e.g., lipids) possess weak anisotropic diamagnetism, which can be aligned (because diamagnetic susceptibility is additive) in the presence of strong magnetic fields (>8 T). The development of warm-bore (−100°C–300°C) vertical- and horizontal-field superconducting magnets will greatly expand the influence of static and dynamic soft matter neutron scattering studies and open up a previously unexplored science direction.

3.4.1.3 Hydrostatic Pressure

Pressure is an important thermodynamic variable, and in many cases it is equally as important as temperature. Importantly, the effects of pressure and temperature on systems are not the same. Specifically, a pressure change affects the system's volume, whereas a temperature change affects both its energy and volume. For example, hydrostatic pressure can be used to study the molecular interactions that cause a protein to adsorb to a membrane surface, as well as how protein–protein interactions occur on the membrane surface. Moreover, for soft materials in water, pressure provides a means of separating the effects of volume and temperature on their phase behavior. The development of reliable pressure cells capable of hydrostatic pressures greater than 400 MPa will significantly affect static and dynamic soft matter neutron scattering studies by accessing phase space that cannot be achieved via temperature changes.

3.4.2 High Magnetic Fields and Low Temperatures

Measurements utilizing magnetic fields and low temperatures are performed on a majority of ORNL beamlines to provide the required tuning parameters for scientific discovery. These measurements are particularly significant for quantum materials but extend to chemistry, biology, and engineering. Developing an understanding of quantum materials for information and energy, as described in Section 2.1, requires measuring materials at extremes of temperature and magnetic field. To attain this understanding, ORNL has can achieve 0.05 K and 14 T, with options for combining other parametric controls. To meet these scientific goals over the next 10 years and beyond requires pushing the extremes by adding new capabilities and efficient equipment operation.

3.4.2.1 Increase Capability and Experiment Capacity

Currently, demand for neutron experiments with magnets is beyond the capacity for beam time, and highly rated experiments are being turned down. Furthermore, the increasing scientific and technical complexity of experiments is driving the need for specialized magnet and low-temperature equipment that leverage the capabilities of specific beamline characteristics, such as solid-angle coverage or polarized setups. To meet this capacity and complexity challenge, the number of magnets must increase. Realistically, given the expense of magnets, the number of magnet investments in the next 10 years is limited. Therefore, the first magnet investment is a multi-instrument magnet at HFIR, followed by magnet investments tailored for a small subset of instruments at both HFIR and SNS. Priority magnet acquisitions include the following:

- A 6 T vertical field magnet for HFIR is the first step to address current capacity limitations at HFIR.
- Horizontal fields magnet capabilities are extremely limited at HFIR/SNS, which means that some important experiments cannot be supported. Addressing this limitation requires a shared horizontal field magnet (3–5 T) for the triple-axis instruments at HFIR and a second magnet at SNS for CNCS (BL-5)/HYSPEC (BL-14B).
- A large vertical divergence magnet for CORELLI (BL-9), ARCS (BL-18), and SEQUOIA (BL-17). This magnet would leverage the large vertical acceptance (±20°) of these instruments and optimize tail design for minimum background owing to multiple scattering.

- A dedicated magnet for half-polarized neutron diffraction at HFIR with the modest field requirements of 3 T. Such measurements are performed on DEMAND (HB-3A) and POWDER (HB-2A) for an ever-increasing percentage of beam time.
- A 15 T split-coil field vertical magnet to enable the new science capabilities of the proposed MANTA instrument.

3.4.2.2 Ultrahigh Steady-State Magnetic Field Investments

The use of high-temperature superconducting (HTS) materials has recently enabled dramatic increases in available field magnets for nuclear magnetic resonance (from 23.4 to 28.2 T) and condensed matter physics (from 22 to 32 T). Now is the time for a similar increase from the 15 T magnet available for neutron scattering, enabling higher steady-state fields without the additional infrastructure and energy required to operate resistive magnets. However, each purchase is a multiyear R&D effort. The market for neutron scattering magnets is small, and any path to enable R&D has been difficult to find. Nevertheless, two magnet developments are proposed: one targeting the highest achievable steady-state field possible for neutron scattering and the other targeting the highly desirable scattering configuration of a vertical-bore split-coil. For both magnets, the following robust strategies are proposed:

- Highest steady-state magnetic field (25 T) horizontal-bore conical-taper no-gap magnet for neutron scattering. This magnet maximizes the steady-state field at sample and simultaneously minimizes risk by avoiding a gap in the HTS coils, thereby approximating a solenoid geometry similar to already operating low-temperature superconducting (LTS)/HTS magnets. For the LTS outsert, options include both a conventional LTS coil and a cable-in-conduit conductor coil design similar to that constructed by National High Magnetic Field Laboratory and operated at the Helmholtz-Zentrum Berlin [11].
- Vertical-bore HTS-only split-coil magnet, maximum field between 16 and 20 T for use at the proposed MANTA and/or HYSPEC and CNCS (BL-5). This magnet optimizes scatter and sample conditions and reflects the relatively much more frequent use of vertical-bore split-coil magnets compared with horizontal-field magnets at neutron scattering facilities worldwide. Given the demand for the newly available 14 T magnet in the user program, an up to 20 T magnet is expected to provide even more scientific impact and demand in the user program.

3.4.2.3 Pulsed Magnets, from Demonstration to the User Program

NScD, in partnership with Professor Nojiri (Tohoku University, Japan), had initial success with pulsed magnets up to 30 T for diffraction [12]. A maximum magnetic field of 30 T is generated every 5 min, and a typical pulse width is 5 ms, which is 30% of the neutron pulse timeframe (17 ms). Subsequently, several other experiments were performed, and an in-house capability was developed to wind coils and integrate them into liquid helium cooled inserts for top-loading liquid helium cryostats. This capability is now mature, with an improved understanding of how to assemble these magnet inserts and will be made available to the user program.

3.4.2.4 Dynamic Nuclear Polarization Magnet

Unlike the demonstration-level dynamic nuclear polarization (DNP) system which requires dilution refrigeration to preserve hydrogen nuclei polarization, this new magnet will enable DNP at a more quickly achievable temperature of 1 K and facilitate faster sample changes. This magnet will be shared between IMAGINE (CG-4D), supporting experiments in the strategic science area of biological materials and systems (Sections 2.5.12.5.1 and 2.5.2) [13], and GP-SANS, (CG-2) supporting experiments in the strategic science area of polymers (Section 2.2) [14].

3.4.2.5 Operations

Areas of operations under high magnetic fields and low temperatures where anticipated improvements align with long-term goals include the following:

- Helium recovery and recondensing. Much of the low-temperature and high-magnetic field capabilities require helium, and the need for investing in such systems is well recognized [15]. Without helium recovery and recondensing, the costs to maintain the current mode of operation may become unfeasible.
- Automation in sample changing at extreme conditions. A current experimental bottleneck is sample change time, which can take several hours. Multisample environments have been extended to less than 1 K on specific beamlines that allow switching between samples in seconds. Developing pathways for widely available multisample changers at low temperatures and high magnet fields will increase productivity, relieve the burden on staff, and enable further remote experiment options.
- AI/ML driven parameter changes. Data-driven temperature changes and stabilization will streamline experiments by smart monitoring and feedback of temperature/field to the data collected. Proof-of-principle measurements have been used to efficiently follow magnetic transitions on WAND2 (HB-2C), pointing to future development opportunities.

3.4.3 High Pressures

The high-pressure research effort at ORNL is a multifaceted program that involves a broad range of research directions. This effort is facilitated by extensive expertise in a wide range of high-pressure science and technologies as well as a variety of recent cutting-edge developments that have been achieved in-house. The results of these efforts are making ORNL a leader in high-pressure neutron scattering, a position that can be maintained through continuous future development, addressing the needs of the science community.

To achieve this leadership status, a large range of high-pressure cells is used and developed across the facilities. For example, gas pressure cells, limited to approximately 0.6 GPa, allow for large sample volumes and are often used for in situ chemistry or the study of samples with weak magnetic moments and/or complex crystallography [16]. Special gas/liquid pressure cells and setups are used for SANS studies on geological [17] or biological [18] materials. Furthermore, clamp cells that allow pressures to 2 GPa are commonly used in studies focused on quantum materials because they can be easily combined with ultralow temperatures, high magnetic fields, and can allow in situ pressure monitoring [19]. Another mainstay is the Paris-Edinburgh cell ([20] and references therein) that enables pressures up to approximately 20 GPa at ORNL. It is predominantly used for diffraction, but uses are currently being expanded to quasi-elastic scattering [21] and inelastic neutron scattering. Additionally, significant efforts have been made to develop diamond anvil cells for neutron scattering. Versatile cells limited to approximately 10 GPa are available for neutron spectroscopy and single crystal diffraction [22][23], and current developments aim to enable simultaneous ultralow temperature and pressure using these cells. Finally, considerable effort has been made to expand to the megabar (100 GPa) regime that is standard for optical methods. Cell development continues with previous cell designs [24], enabling refinable data quality up to approximately 60 GPa [25]. Recent progress now also enables high-pressure research on super hydrides [26] and has finally broken the megabar barrier.

Although these existing capabilities enable a large range of research directions, several new critical capabilities will be required to address the future needs of the strategic science areas detailed in Section 2. These new capabilities can be loosely grouped into two categories. In the first category, high pressure is applied in a truly hydrostatic manner and is consequently often regarded as a clean tuning parameter. Most neutron user experiments within the strategic science area of quantum materials, as detailed in

Section 2.1, are conducted in this manner, although pressures are limited to below 10 GPa. In the second category, above approximately 10 GPa, pressures become nonhydrostatic, the details of the experiment significantly influence results, and the scientific question cannot be considered independent of the experimental setup. This pressure regime is required for many science questions falling into the strategic sciences areas of chemistry, geochemistry, and environmental sciences (detailed in Section 2.4) and materials and engineering (detailed in Section 2.3). The strategic science area of quantum materials (Section 2.1) also requires such conditions in the quest for the stabilization of exotic phases of matter, and the strategic science area of soft matter and polymers (detailed in Section 2.2) benefits from such in situ extremes in the upcycling of polymers. To tackle science questions in both categories, several new capabilities will be required.

A particular need for the strategic science area quantum materials centers on the application of multi-extremes, particularly high pressure, high magnetic field, and ultralow temperatures. These powerful tuning parameters provide unique insight into the many-body physics of correlated electrons and can aid in understanding, and hence controlling, quantum fluctuations as necessary for novel quantum materials for energy (Section 2.1.2). Applying such multi-extremes requires developing cells with sufficiently nonmagnetic properties (even once pressurized), setups that avoid beam heating of the sample, and magnets with sufficiently large bores. Although cell designs can be developed in house, a true extension of capabilities toward this combination of extreme environments will most likely require close collaboration and co-development with magnet experts from facilities outside of ORNL.

By contrast, the simultaneous application of high pressure and high temperature is required for several of NScD’s strategic science areas. For example, the Haber-Bosch process for ammonia production (Section 2.4) is regarded as the first technological application of a high-pressure, high-temperature synthesis. Higher pressures and temperatures are required to further understand phase transitions relevant to this strategic science area. Furthermore, future upcycling of polymers (Section 2.2.2) requires in situ neutron probing of materials under extreme conditions. Similarly, high-pressure, high-temperature conditions can yield the synthesis of new materials that better withstand harsh conditions and can be used in turn to probe the resistance of durable materials (Section 2.3.2). Finally, high pressure and high temperature are also required for the synthesis of novel quantum materials for energy (Section 2.1.2) such as high-pressure super hydrides with their high T_c superconductivity for improved energy transmission. The necessary high pressures and temperatures above 1,000 K must be achieved via laser heating in a diamond anvil cell. Initial developments can thereby focus on ex situ laser heating (i.e., a sample is heated while under a given pressure in order to synthesize a desired material, for example, more durable) the resistant materials. Furthermore, specifically in super hydride research for better quantum materials for energy, new methods are required that enable such processing in the presence of hydrogen loaded into a diamond cell. Ultimately, development of in situ laser heating in a diamond cell on a beamline will be required to observe in situ high-pressure, high-temperature conditions. Although such ex situ and in situ laser heating has not been deployed yet for neutron scattering, the technique is well established for optical diamond cells, and in-house expertise exists to adapt the technique to neutron scattering.

Finally, across the entire suite of cells, expansion beyond the current pressure limit is required. For example, the arrival of a new 1 GPa gas intensifier is imminent, so development of 1 GPa gas pressure cells will be required within the next few years. Gas pressure cell development includes not only cylindrical cells for diffraction or inelastic scattering but also special cell designs used for SANS or QENS that are relevant to chemistry, geochemistry, and environmental sciences, and soft matter and polymers. Furthermore, cell concepts are required that enable similar sample volumes as present in the clamp cell yet allow for pressures to approximately 10 GPa. This capability would open many new avenues for quantum materials research across the SNS and HFIR instrument suites, especially on instruments for which the sample volume allowed by the diamond cell is too small. Finally, pushing the pressure limit well beyond 1 Mbar (100 GPa) will be critical to enable access to the pressure regimes required for synthesis of materials that can withstand harsh conditions or of new super hydrides. Whereas this latter push will clearly benefit from additional facility power available after the PPU, it will also require investment and research on incident-beam and/or radial collimation and instrumentation itself.

Overall, ORNL boasts the expertise to tackle many of these developments (with perhaps the exception of the codevelopment of high pressures in high magnetic fields). Such development does, however, require significant time investment, staff time required to develop but also time on beamlines to develop, test, and ultimately commission these exciting new capabilities. With these investments in place, ORNL will be able to maintain its position as a leader in high-pressure neutron scattering.

3.4.4 High Temperatures and Levitators

The diverse science targeted in Section 2 requires accurate, repeatable, user friendly, and safe temperature control throughout a variety of regimes. To this end, the high temperature sample environment team develops, deploys, and maintains a wide suite of conventional furnaces, closed cycle refrigerators, unique levitation furnaces, and beamline-specific systems, with applications ranging from routine high-throughput studies performed a few hundred degrees above ambient temperature to unique in situ experiments above 2,000°C. At moderate temperatures, the reaction pathways and catalysis processes described in Section 2.4 are observed in situ using carefully controlled atmospheres in specialized furnaces. In service of the priorities outlined in Section 2.3.1, the microstructural development of new alloys for additive manufacturing can be probed under synthesis and service conditions, which is critical for the selection of the next generation of candidate materials, while at the same time optimizing directed energy-deposition processes that require environments designed for the in situ study of materials undergoing nonequilibrium processes at high temperatures. Apparatus for containment and temperature control at higher temperatures enables the study of the structure and dynamics of molten salts, critical to the aims described in Section 2.3.2, and enables compositionally complex alloys envisioned as structural components of or cladding for nuclear fuels to be probed at relevant real-world conditions. Finally, the development of the next generation of promising structural materials for engineering technologies, such as high-entropy ceramics, or the study of key reactor components, such as nuclear graphite, require extreme temperatures (>2,000°C) currently incompatible with conventional neutron scattering furnaces and crucibles, necessitating advanced techniques such as levitation processing for in situ study.

In accordance with this broad responsibility, NScD's priorities over the next 10 years will be grounded in four target areas: (1) increasing operational efficiency and automatability; (2) improving control and metrology; (3) expanding the range of compatible materials and temperatures by using novel setups such as levitation technique, new heating methods, and beamline-specific developments; and (4) enabling multimodal in situ study of synthesis and reactions on the beamline.

First, by capturing and analyzing electrical characteristics of furnace heating elements during long processing cycles, will allow for using ML to predict and prevent element failures in conventional furnaces, reducing downtime and increasing efficiency. Beam time efficiency will be increased by offering rapid heating and cooling rates, using methods such as rapid gas cooling of conventional furnaces as well as techniques such as rapid sintering via novel carbon heating elements and laser heating. Additionally, the possible space will be expanded for additively manufactured materials, as outlined in Section 2.3.1, for which rapid heating/cooling rates and significant thermal gradients are necessary to accurately reproduce operational conditions. Sample-changing capabilities at high temperatures will be developed and introduced, enabling autonomous experimentation as flux continues to increase as a result of investments such as PPU and STS.

Second, because accurate thermometry is critical for replicability and the linking of computational and experimental results, improved temperature measurement schemes, including fiber optics, multiwavelength pyrometry, and in-house calibration schemes, will be deployed to improve sample temperature measurements and to characterize gradients in furnace temperatures across all regimes, reducing measurement uncertainties. Alternatives to current control schemes, including autotuning proportional-integral-derivative schemes and AI assisted controls, will be investigated both for finer control on the beamline and to lessen staff intervention.

To provide the conditions experienced by ultrahigh-temperature ceramics, compositionally complex alloys, and reactive molten salts in demanding structural and nuclear applications as described in Section 2.5, the levitation suite for containerless processing will be continually improved. By applying pressurization for volatile materials, the temperature ceiling of NScD's containerless processing capabilities will be raised, enabling the study of important materials such as nuclear graphite and fluoride salts. For more conventional furnaces, NScD will pursue new sample containment, including materials like null-matrix alloys and ultrahigh-temperature ceramics, as well the use of alternate manufacturing and procurement, such as 3D printing.

Finally, deploying in situ characterization techniques, such as noncontact physical property measurement, Raman spectroscopy, and resonant ultrasound spectroscopy, in combination with structural and dynamical neutron scattering measurements, will enable full characterization of high-temperature synthesis and reaction pathways on the beamline, which is critical for understanding the processes laid out in Section 2.4 and for advancing design paradigms for the materials in Section 2.3. Enabling the user community to test samples in NScD's unique levitation systems before beam time and acquiring complementary physical property measurements will expand the high-temperature user community and strengthen the pipeline of scientific output. Thermomagnetic processing and the application of magnetic fields during thermal processing supports the broader goals of Section 2.3 by providing more energy efficient routes to the creation of manufacturing alloys. Similarly, enabling combinations of temperature with other extremes, such as field, electrochemical potential, or atmosphere, will allow for simulating real-world conditions of synthesis and service. In pursuit of this goal, beamline-specific systems will be prioritized to enable new science, such as compact furnaces at MARS (CG-1D) and SANS beamlines to enable characterization across time, length, and energy scales.

3.4.5 Sample Preparation and Complementary Techniques

The needs for sample preparation and complementary techniques for characterization vary considerably among the diverse scientific domains to which neutron scattering techniques are applied. The strategic approach of the HFIR/SNS neutron user facilities is to provide laboratory facilities that are adequate to maintain the broad diversity of neutron scattering applications, which include scientific domains as dissimilar as solid-state physics, materials science and engineering, and biology. The operational model of HFIR and SNS, as DOE BES user facilities, relies on external users to provide their own materials synthesis and characterization before performing neutron scattering experiments. With that requirement understood, essential sample preparation and complementary techniques are provided on-site when necessary. Most of these facilities are an integral part of the HFIR/SNS user facilities. Additionally, the Neutron Scattering Division maintains partnerships and collaborations with other user facilities, benefitting the scientific user community at large. Especially notable are collaborative agreements with the collocated Center for Nanophase Materials Sciences (CNMS, a DOE BES user facility) and the Center for Structural Molecular Biology (a DOE Biological and Environmental Research user facility). The following is an overview of sample preparation capabilities and complementary techniques that are maintained for the support of the neutron scattering user program at HFIR and SNS. The NScD website (https://neutrons.ornl.gov/lab) provides further details.

3.5 Technological Developments

The importance and significance of technology developments for neutron scattering instruments are demonstrated by at least an approximately 1,000-fold increase in instrument performance since the early 1970s—depending on the metrics used for performance, the case for an even greater gain factor could be made. In the same time span, the time-averaged brightness of neutron sources has not increased, but pulsed sources now offer high-brightness pulses and a time structure of the beam that can be exploited. Technology areas that have seen huge performance increases include beam transport systems (guides), detectors, polarization analysis, pulsed beam operation (choppers), data acquisition, and data storage.

The following three subsections summarize planned neutron technology developments at ORNL in the areas of neutron detectors, beam polarization devices, and new moderator materials. These developments are driven by user demand and scientific discoveries and are being realized through close collaboration between facility staff and the user community. Facilities must anticipate development directions and provide the infrastructure to enable technology developments.

3.5.1 Detectors

Detectors are critical components needed in scattering facilities. Their continued development is essential to operating world-leading instruments for materials science and engineering. This section highlights plans for neutron detector development in four critical areas where gaps or unmet instrument needs are observed.

Neutron scattering instruments at ORNL require the recording of an image of the neutron signal in 1D, 2D, or 3D. Neutron detectors are required to operate under high neutron brightness, with high position resolution (sub millimeters to a few micrometers), with excellent position linearity and stability, with electrical stability, with high count-rate capability, and with insensitivity to gamma background.

Most of the current detectors at ORNL meet the requirements of the various instruments; however, four detector technologies need further development to better meet the desired instrument specifications. Figure 3.5-1 summarizes current detector performance and the targeted performance for these four detector technologies:

- **Improve spatial resolution.** The new generation of scintillator-based detector technologies will improve the spatial resolution by developing brighter and faster scintillators to enable more challenging science. These improvements will primarily benefit applications in powder and single-crystal diffraction, which are innovative avenues of research in pursuit of superior materials and understanding of biological processes involved in human diseases. For example, complex structural details in new materials under investigation as catalysts (Section 2.4) or as metal organic frameworks (Section 2.2) may be much more directly accessible with improved resolution detectors. Similarly, subtle structural rearrangements associated with phase transitions in quantum materials (Section 2.1) will become observable.
- **Increase count rate capability.** Fast (nanosecond time resolution), high dynamic-range detectors ($>10^{+8}$) that are insensitive to gamma rays ($<10^{-7}$) will be needed for neutron reflectometry and small-angle scattering, which are used to study nanostructures and magnetic properties at surfaces and interfaces. Detectors with such features will enable the performance of complete reflectometer experiments on nano systems. Complete reflectometry includes TOF reflectometry, off-specular scattering, and grazing-incidence SANS geometry in one shot. An increased dynamic range in a detector will be of interest to soft matter science (Section 2.2) for which the scattering often strongly varies with Q in a narrow range covered simultaneously in an experiment.

- **Improve imaging detectors.** Detector technology to meet requirements for advanced neutron imaging (Bragg edge imaging, resonance imaging, wavelength-dependent grating interferometry, and polarized imaging) will be critical for supporting materials and energy research. These detectors will require high position (micron) and timing (nanosecond) resolution capabilities to accurately record the 2D radiographs of all scattering and reaction processes occurring in a sample. The detection system's spatial and temporal resolutions are the critical parameters defining the accuracy of wavelength-dependent neutron transmission measurements needed for obtaining the stress distribution, microstructure, nano- to mesoscale defects, magnetic domains in advanced materials, electrode chemistry and performance in lithium batteries, and water distribution in plants and fuel cells.
- **Better beam monitors.** Neutron beam monitors are low-efficiency detectors in which only a fraction (approximately 1%) of the incident beam is absorbed or scattered; the remainder is transmitted. Beam monitors are an important diagnostic tool in neutron facilities because they monitor the neutron flux, beam distribution, and pulse timing to ensure that the beam conditions reliably conform to what is expected. They also provide information about the beam flux that is necessary to normalize scattering data. Higher speed detector technologies are therefore needed to address the current counting rate limitations in many instruments. The future generation of neutron beam monitors should provide fast time resolution (sub-nanosecond), provide very strong gamma ray rejection, and be position sensitive for beam profiling. AI/ML techniques indicate that great potential exists for the additional information captured by monitors during an experiment to be used for adaptive instrument control (Section 2.3).

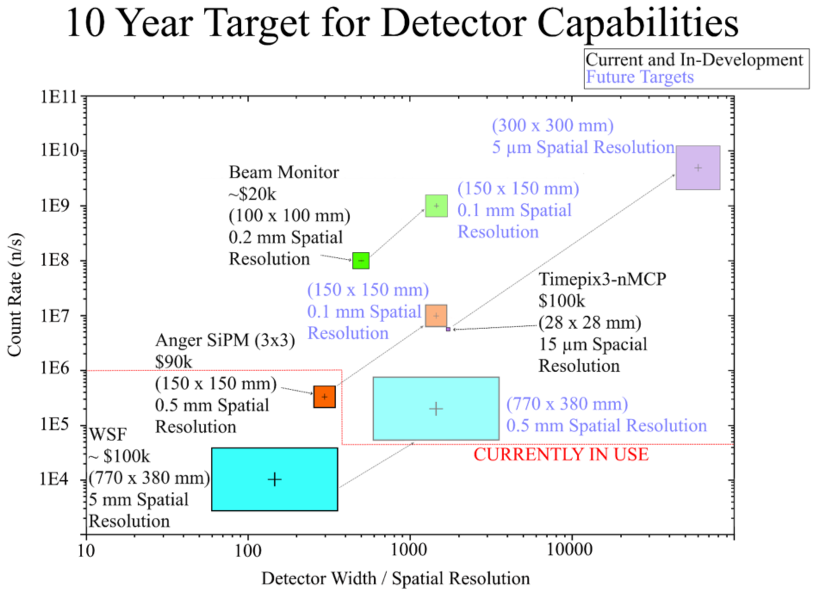


Figure 3.5-1. 10 year target for detector capabilities In the chart (in which the size of box symbol is proportional to the area of the 2D detector), detectors (below dashed red line) in use at SNS and HFIR are situated at the bottom, signifying low count rate performance. The required performance of each of the four proposed detectors is labeled as future target by 2030.

Parameters that will be considered when choosing the next generation detector technology are spatial resolution, distortion, efficiency, count rate, gamma sensitivity, uniformity, and active area.

Table 3.2. Operational targets for the detector technologies described for the next decade.

	Resolution (FWHM*)	Distortion	Efficiency (2Å)	Counting rate (counts/s)	Gamma (^{60}Co)	Active area (cm^2)
Powder Diffraction	0.5 × 2 mm	—	>70%	2.0×10^5	$<1 \times 10^{-6}$	30
Single Crystal	0.1 mm	<0.05 mm	>65%	5.0×10^6	$<1 \times 10^{-6}$	225
Reflectometer	0.5 mm	—	>65%	5.0×10^6	$<1 \times 10^{-6}$	400
Beam monitor	0.1 mm	—	10^{-5}	1.0×10^8	$<1 \times 10^{-6}$	225
Imaging	5 μm	—	>50%	5.0×10^9	$<1 \times 10^{-6}$	900

*FWHM = full-width-at-half-maximum.

3.5.2 Neutron Polarization

ORNL has a long history in developments and research involving polarized neutrons. Shull et al. first demonstrated that highly polarized neutron beams are obtained for certain reflections of magnetized iron and Fe_3O_4 crystals at ORNL's Graphite Reactor [27]. The neutron polarization analysis technique was first developed at HFIR [28][29] in the 1960s, and important developments in supermirror polarizers were made in the 1980s [30][31]. Neutron polarization continues as an essential element of neutron instrumentation at HFIR and SNS. Although many of the polarization techniques currently used are best suited to the continuous beams available at HFIR, demand at SNS (especially for future STS instruments) is increasing. The demand for polarized neutron applications will increase in the next 10 years in the following three general areas.

- Polarization analysis of scattering from magnetic structures within samples: polarized neutrons interact with the polarization state of the sample, leading to better understanding of magnetic structure and dynamics.
- Larmor labeling techniques: the neutron moment is used as a timing mechanism for the neutron flight path, allowing measurements of very small changes in the neutrons' velocity or direction.
- Nuclear spin–dependent neutron scattering: the interaction of the neutron with the nuclear spin can be leveraged to improve the signal-to-noise ratio in diffraction measurements, extract structural information, or discriminate between coherent and incoherent scattering.

The following subsections outline the goals for neutron polarization developments over the next 10 years:

3.5.2.1 Spherical Polarimetry at HFIR and SNS

The earliest polarization analysis measurements, by Moon [28] and others, analyzed scattering in 1D, with the understanding that the interaction between the neutrons and the sample is 3D. Spherical neutron polarimetry (SNP) was pioneered by Tasset et al. [32] with the Cryopad apparatus at the Institut Laue-Langevin. More recent innovations [33] led to aims to use high-T_c superconducting thin-film technology to build an innovative portable SNP device, deployable at multiple ORNL instruments to enable measurement of off-diagonal elements of the polarization tensor. This research is the subject of a DOE Early Career Award project let by an ORNL Neutron Optics and Polarization Group staff member. This device is expected to be available soon for the user program at the PTAX (HB-1) polarized triple-axis spectrometer at HFIR. The apparatus should be readily adaptable to the future MANTA cold triple-axis spectrometer at HFIR (to be built as part of the HBRR Project—Section 3.2.4.3), as well as SANS or diffraction instruments. An additional effort is underway to adapt the technique to TOF instruments at SNS: initial efforts focus on the HYSPEC instrument (BL-14B). SNP development is an enabling technology for the strategic science area of quantum materials (Section 2.1).

3.5.2.2 Development of Beam Polarization Techniques

Neutron polarization filters include polarizing crystal monochromators, such as the Heusler units used at PTAX and HYSPEC, polarizing supermirrors, and ^{3}He transmission filters. The crystal devices are limited to monochromatic beam instruments. Polarizing supermirrors, which work well as polarizers for longer wavelength instruments, have become available commercially; the Neutron Optics and Polarization Group continues to help with supermirror selection and device design for individual instruments.

The Neutron Optics and Polarization Group has an established program using spin exchange optical polarization technology to polarize ^{3}He. The team fabricates new cells and supports their use at the instruments. Drop-in cells are prepared in a laboratory, and then they can be polarized and moved to beamlines. In the last few years, the group has developed in situ ^{3}He systems for multiple instruments, including MAGREF (BL-4A) and DEMAND (HB-3A). The in situ systems have been demonstrated on other instruments, particularly at HFIR, including on the triple-axis spectrometers, MARS (CG-1D), and the SANS instruments. The in situ cells allow constant polarization measurements, unlike drop-in cells that have a limited polarization lifetime, allowing more straightforward data acquisition and analysis. Additionally, adiabatic fast passage flipping is available in the in situ systems, eliminating the need for a separate flipper. The group intends to build upon this expertise to allow use of more ^{3}He polarizers across the ORNL neutron instrument suite and to make these devices more robust for routine use. Polarizing optics are an enabling technology for the strategic science areas of quantum materials (Section 2.1, for magnetic studies), biology materials and systems (Section 2.5, with DNP to improve structural determinations of proteins), and materials and engineering (Section 2.3 for polarized neutron imaging).

3.5.2.3 Neutron Larmor Techniques

The neutron spin precesses at a rate governed by the strength of the local magnetic field, known as the Larmor frequency. In effect, the neutron precession phase is governed by its path through the field, which allows the neutron precession to serve as a very sensitive timer for the neutron. NSE spectroscopy was the first successful use of this property [34][35] for neutron scattering measurements. Development has continued on such techniques, and recently the effort at ORNL has increased. Several demonstration experiments have been conducted [36][37][38][39], and a system, mainly developed by NScD's staff, uses neutron Wollaston prisms for high-resolution inelastic scattering and diffraction measurements. At this time, the system has been used on the development instruments HB-2D and CG-4B at HFIR, but the most effective use has been on the PTAX polarized triple-axis instrument. A DOE Early Career Award project is being led by an ORNL Neutron Optics and Polarization group staff member to conduct high-resolution measurements using the Wollaston prisms and related Larmor techniques with an intent to make the technique available to a wider community. The succeeding plan is to make these Larmor methods usable on cold instruments such as the future MANTA triple-axis spectrometer at HFIR (Section 3.2.4.3), SANS instruments at HFIR, and possible future SNS TOF instruments. This capability will be in addition to the planned HFIR-NSE instrument to be developed at HFIR, a part of the HBRR Project. Larmor techniques support the strategic science area of quantum materials (Section 2.1) because they allow scattering to be observed with much better resolution than is possible with standard diffraction techniques, and they support the soft matter and polymers (Section 2.2) and biological materials and systems (Section 2.5) strategic science areas, which require the use of NSE spectroscopy to measure slow dynamical processes.

3.5.2.4 Dynamic Nuclear Polarization

DNP is a method to polarize nuclei within a sample. This technique, combined with polarized neutrons, provides in situ control of the neutron cross section, and could provide up to 1,000-fold gains in performance for diffraction analysis of hydrogenous materials. A prototype apparatus to develop DNP of hydrogen nuclei, constructed by the Neutron Optics and Polarization Group, has been operated at the IMAGINE quasi-Laue diffractometer (CG-4D) for a series of trial measurements since September 2017 [40]. These proof-of-concept measurements have demonstrated significant enhancements to the diffraction measured from protein single crystals. This technique can be realized on a reconfigured IMAGINE beamline or at STS (on the PIONEER instrument for example) using a new production-capable DNP system. DNP may be used separately or in combination with deuteration for contrast enhancement in a variety of hydrogenous materials. DNP has clear applications in the strategic science areas of biological materials and systems (Section 2.5) [13] and has potential for use with soft matter and polymers (Section 2.2) [14].

3.5.2.5 Wide-Angle Polarization Analysis

Large-area detectors are common at spallation sources, including the SNS FTS and STS (where several of the instruments in the initial suite, such as CHESS and EXPANSE, require full polarization analysis in a detector with large out-of-plane and angular coverage). Although technical solutions exist for the problem of wide-angle analysis, the scale—in terms of the size of the area to be covered and the number of instruments—is unprecedented at ORNL. Development of efficient and cost-effective analyzer schemes will be essential to the success of these instruments.

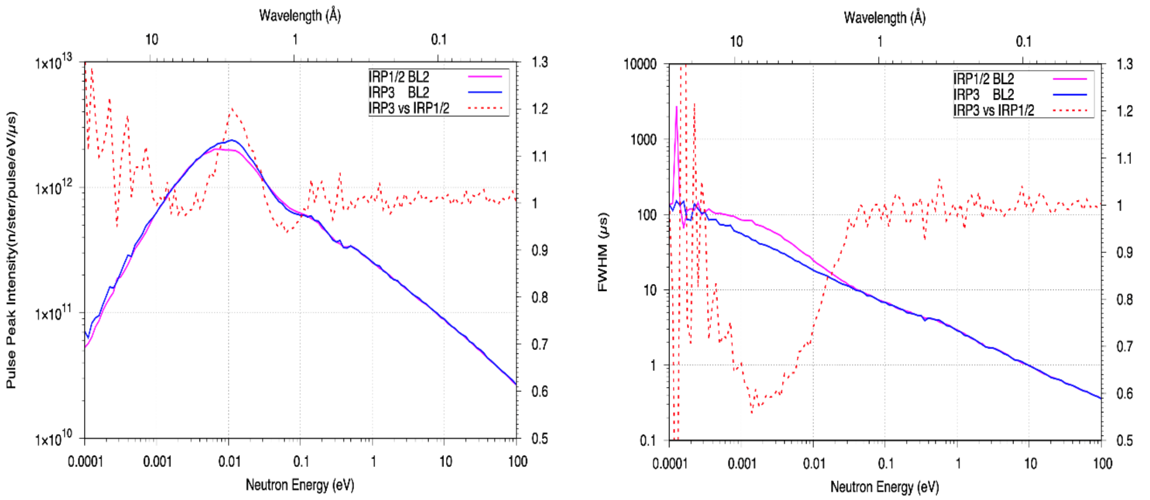
3.5.3 Moderator Developments

The developments described in this section are relevant for most, if not all, instruments at SNS. All science areas covered by these instruments (Section 2) will benefit in various ways from improved source stability and sharpened source pulses.

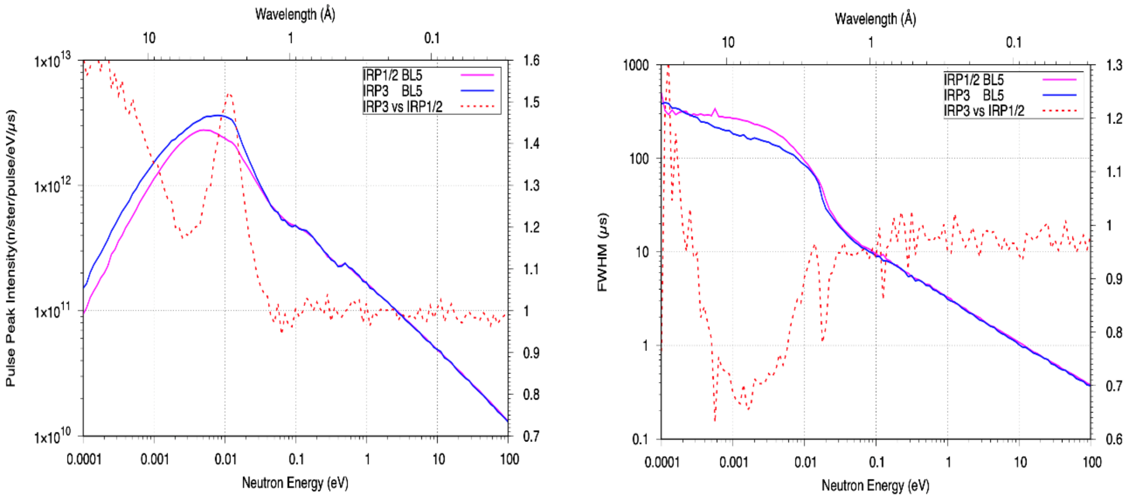
3.5.3.1 Proton Power Upgrade Effect on Moderator Performance

The PPU Project's primary goal is to enhance neutron production by increasing the power into FTS from 1.4 to 2 MW without changing the existing SNS moderators. The proton energy increase yields a 10% increase of the neutron brightness of the downstream coupled-hydrogen moderators because the neutron production zone moves slightly downstream.

Another significant PPU effect on moderator performance will be the implementation of IONEX catalytic converters in the hydrogen loops. These converters will counter the week-long relaxation times into the para ground state after filling the hydrogen loops and the power-driven back-conversion into the ortho state experienced in the present system. The present system is operating with the power-dependent equilibrium mixture, which at approximately 1.4 MW power, consists of approximately 30% ortho- and 70% parahydrogen. Figure 3.5-2 depicts the expected moderator performance after the PPU completion compared with the present system in terms of pulse peak intensity (both assumed at 2 MW), and the full-width-at-half-maximum (FWHM) pulse width for the two types of SNS hydrogen moderators: the decoupled poisoned and the coupled ones. For both hydrogen moderators, strong narrowing of the pulse shapes in the thermal and cold energy ranges is expected at increased pulse peaks. Narrower pulses improve the energy resolution of the neutron scattering instruments and align FTS with the three-source strategy because high resolution will allow FTS to continue to excel in a post-STS world.



(a) Decoupled poisoned hydrogen moderator



(b) Coupled hydrogen moderator

Figure 3.5-2. Peak pulse intensity and FWHM pulse width of SNS hydrogen moderators in present state (inner reflector plug (IRP)-1 and IRP-2) and after PPU Project (IRP-3). The red dashed line shows the ratio PPU/present on the right plot axes.

3.5.3.2 Inner Reflector Plug Developments

Within a 10-year period, FTS will exhaust the inner reflector plugs (IRPs) IRP-2 and IRP-3 (start of service in CY 2025) and will be approaching IRP-4's end of life (projected for CY 2033) as outlined by the IRP Management Plan shown in Figure 3.5-3. Because the life cycle of an IRP throughout design, manufacturing, and service is about 8–10 years, changes to an IRP (e.g., a change of a moderator characteristic in response to changed instrument requirements) need long-term planning. Within the coming decade, the SNS FTS instrument suite changes will focus on the build-out of the remaining open beamlines. Therefore, a demand for a big moderator change is not expected within this timescale. However, the STS Project will be approaching the start of neutron production in not much more than 10 years. The STS project will bring eight new instruments and launch ORNL into the three-source era. To ensure good FTS–STS complementarity, we should start considering how to modify the FTS. For example, we must consider which moderators may replace the FTS coupled moderators and which new spectral characteristics they will offer.

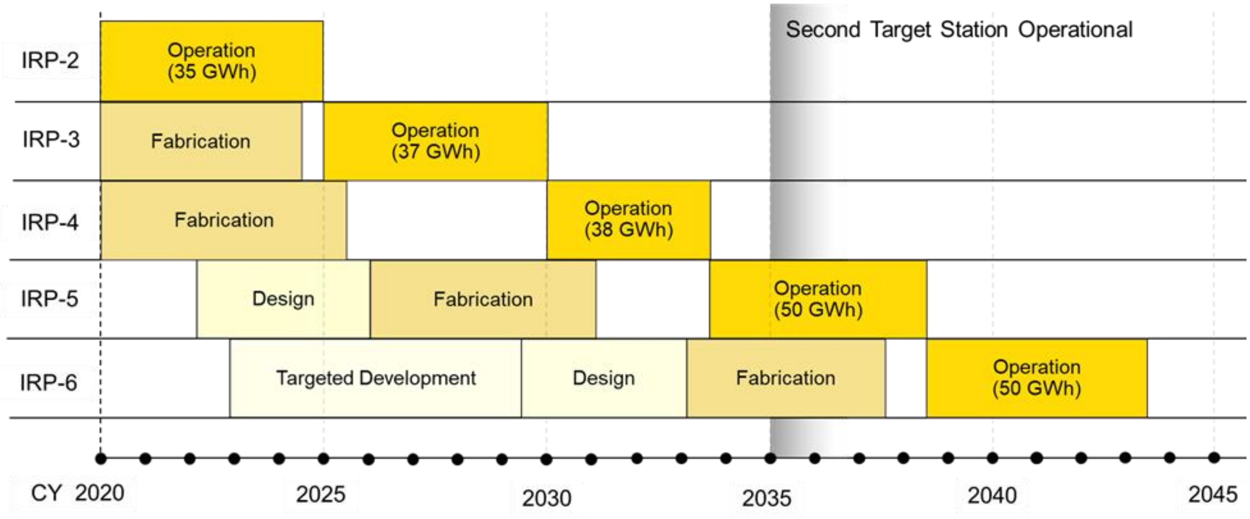


Figure 3.5-3. Schedule for development, design, fabrication, and operation of inner reflector plugs through IRP-6.

Since the initial design of the FTS, new moderator concepts have been developed, such as low-profile higher brightness moderators, that have the potential to increase the performance of the FTS. Also, a moderator with alternative characteristics to the decoupled poisoned liquid hydrogen and water moderators is of interest. Although a decoupled hydrogen moderator would lean toward the strengths of the FTS relative to the STS, other options exist. A liquid ammonia moderator operated at 190 K offers a spectrum that lies between those of hydrogen and water. It is a very attractive candidate for high-resolution applications because of the faster moderation owing to hydrogen's higher density compared with water. Using ^{15}N-enriched ammonia will lower the losses of neutrons to absorption in nitrogen and boost performance. However, significant development is needed for such a system, including the verification of ammonia's radiation tolerance. Such a significant change to the moderators could be brought to service with IRP-6 in CY 2038. However, this change will require targeted development to identify the path forward and convert the ideas into moderator and reflector systems that can be fabricated and operated reliably. This effort must also be coordinated with changes to instruments to ensure the changes result in new scientific capabilities or improved output.

Beyond IRP-6, there are several other opportunities for development. Alternative ways for poisoning and decoupling should be investigated because increasing the absorber thicknesses will further reduce pulse intensity. Developing liquid neutron absorbers that can be flushed out periodically could solve this problem and regain 25% of neutron intensity to the instruments as parasitic neutron absorption in the epithermal energy range is reduced. Furthermore, the Al-6061 alloy's radiation-damage limits should be explored to possibly extend the IRP lifetimes beyond 50 GWh.

3.5.3.3 Moderator Test Station

The Moderator Test Station (MTS) is planned to be designed and built in the next 4 years. A requirements document has been finalized and a conceptual layout completed shown in Figure 3.5-4 that outlines the scope for building the MTS at the existing beam test facility (BTF), which currently operates a 2.5 MeV proton beam. The existing BTF beamline will be modified to deliver the proton beam to a neutron-producing target within the MTS. Neutrons produced will be prototypic in time structure to FTS and STS and will offer the space and environment needed for moderator development by placing candidate moderator and reflector assemblies near the target. A suite of data acquisition instrumentation and software, including detectors and beam monitors, will be installed to study the effects of any moderator configuration for optimization of both physical and operational characteristics of the moderators.

MTS will be instrumental in validating new STS hydrogen moderator designs as well as researching and optimizing new moderator concepts for future performance gains for FTS. Critical moderator characteristics and operating parameters—such as hydrogen moderators at varying pressure and temperature conditions entering the supercritical phase—can be studied to understand dynamical effects and their influence on moderator performance.

Other novel moderator concepts of interest to FTS and STS may be studied in the future (e.g., low-dimensional moderators, convoluted moderators, pelletized moderators, and ammonia moderators) with the support of a strong moderator development program at SNS.

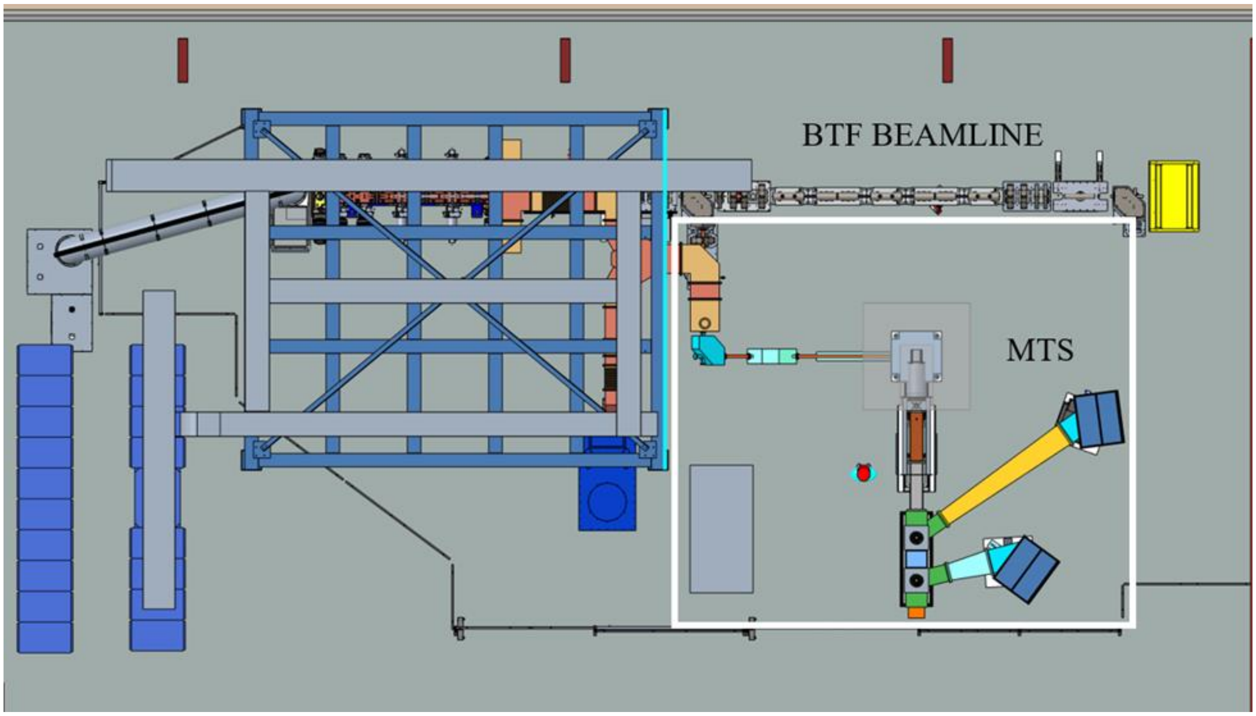


Figure 3.5-4. Moderator Test Station layout at the Beam Test Facility.

3.6 Operational Excellence

Creating a vibrant research environment includes having the staff, the support, and the infrastructure necessary for staff and users to work at HFIR and SNS safely, securely, and effectively. As an integral part of the NScD strategic plan for the next 10 years, this section describes the initiatives and development activities NScD plans to pursue in the areas of workforce development and diversity, equity, and inclusion; career development and work-life balance; the user program; communications; environment, safety, health, and quality; and asset management.

3.6.1 Workforce

This document lays out an ambitious agenda for NScD for the next 10 years. Meeting these goals requires the hard work of a diverse, well-trained, dedicated, and engaged workforce. To this effect NScD is committed to recruiting, developing, and retaining the best R&D and support staff.

Workforce Development and Diversity, Equity, and Inclusion. Diverse teams are always more productive and creative because differences and diverse perspectives lead to the best outcomes. Thus, NScD is committed to recruiting and retaining a vibrant and diverse workforce. ORNL and NScD celebrate the diversity of their employees and their ideas, cultures, and educational backgrounds. ORNL's diversity, equity, and inclusion vision is to create and foster a safe research and work environment in which diversity is essential, equity is inherent, and inclusion is innate. Committing to employees and building an inclusive culture enables and defines NScD's success toward leading the world in research and innovation. ORNL is working to build the future STEM workforce, educating diverse pools of talent with intention and purpose. This goal is achieved through targeted recruitment, creating an environment that is attractive to diverse pools of candidates, and collaboration with minority-serving institutions to strengthen the long-term talent pipeline.

Career Development and Work-Life Balance. To promote a dedicated and engaged staff, it is important to provide development and advancement opportunities, with clear career paths, as well as an environment that is conducive to a healthy work-life balance. This environment will not only promote wellbeing and engagement but also will encourage innovation and unleash the needed creativity for instrumentation development and facility improvements. A recent BESAC subcommittee report on international competitiveness [41] pointed to the importance of providing career advancement opportunities for staff at scientific user facilities. These opportunities are essential to workforce retention and development, and to encouraging innovation. NScD is committed to creating clear and intentional career paths for staff through coaching and mentoring, professional development, and career advancement opportunities.

3.6.2 The User Program

The User Program Office. The User Program Office oversees an integrated program for users of HFIR and SNS. The General User Program is the primary access mode. General user proposal calls are made twice a year, and each proposal receives three or four external reviews from a pool of more than 270 reviewers. Other access modes include mail-in, proof-of principle, and collaborative development. Mail-in programs have been expanded in recent years and currently exist on EQ-SANS (BL-6), NOMAD (BL-1B), POWGEN (BL-11A), SEQUOIA (BL-17), and VULCAN (BL-7).

Joint Proposal Programs. Joint programs with other facilities have also been developed. The Facilities Integrating Collaborations for User Science call allows users to request time at the Joint Genome Institute, the Environmental Molecular Sciences Laboratory, and the BIO-SANS(CG-3) instrument at HFIR through CSMB. A partnership with the CNMS at ORNL allows users to request characterization time within their general user proposal, or to request neutron scattering time in their CNMS proposal. Three HFIR and SNS beamlines (NOMAD [BL-1B], POWGEN [BL-11A], and BIO-SANS) offer programs for users to request x-ray time at one of DOE's light sources as part of their neutron proposal.

Remote Experiments. Remote experiment capabilities were developed during the COVID-19 pandemic to allow more direct access to users unable to travel to the facilities. The work was done on an aggressive time frame as a collaborative effort by many teams across three divisions and included proposal system updates, workflow design, implementation for remote user login, computing hardware purchase and installation at beamlines, beamline control system modifications, user training videos, and interactive messaging tools. These upgrades will continue to support a hybrid mode in which experiment teams include both onsite and remote users.

3.6.3 Communications Strategy

A communications coordinator leads a team of deployed communication professionals to support the directorate in delivering high-quality and timely internal and external communications in web, print, and other media for a broad audience of staff, sponsors, users, and stakeholders, including DOE and partners. The communications strategy aims to increase awareness of NScD's science capabilities, initiatives, research programs, and projects, such as PPU, STS, and HBRR, by promoting neutron sciences in communications with facility users and the public. Communications staff work closely with scientists, leadership, and other support staff to develop and maintain external and internal websites, brochures, features, story tips, science highlights and press releases, graphics, photographs, and videos, and they assist with community outreach. The primary distribution methods for news and updates are the external neutrons and ORNL websites, social media, news releases, feature stories, science highlights, and videos, and a bi-monthly external newsletter sent to approximately 9,000 users. Internally, a weekly internal newsletter and a bimonthly STS newsletter are distributed to more than 1,000 people in the directorate and to laboratory leadership.

3.6.4 Process Excellence

Environment, Safety, Health & Quality (ESH&Q). ESH&Q will continue to support the efficient delivery of the NScD mission while protecting workers, the public, and the environment. A strong safety culture is key to sustaining performance, and work will continue to foster an environment built on trust, respect, and organizational learning, while maintaining a positive safety legacy for staff, users, and visitors. Lessons learned from both internal and external organizations will be applied to improve operational performance. Quality programs continue to support current operations and will support the success of future source and beamline development projects. Periodic assessments are conducted, and performance metrics are monitored by senior management.

Asset Management. SNS completed an Asset Management Improvement Pilot Project during FY 2020–2021 in which rigorous processes were developed and tested in the warm linac portion of the klystron gallery. The project's goal is to increase the entire facility's efficiency and reliability using modern asset management processes by improving reliability management, maintenance workflow management, and spare parts management. The pilot project demonstrated improved work planning, scheduling, and kitting. The asset management project will be implemented for all systems within the SNS facility via a structured process by technical systems.

SNS Accelerator Systems. Long-term strategic plans for the SNS accelerator, including improvements for reliability, obsolescence mitigation, risk mitigation, strategic facility investments, Accelerator Improvement Project (AIP) planning, and strategic R&D directions are described in detail in the Accelerator Management Plan (AMP). The AMP is a living document that is updated annually by the Research Accelerator Division.

Figures 3.7-1 and 3.7-2 represent a tentative high-level schedule for neutron sciences at ORNL for the next 10 years. These timelines are subject to refinement as we gain a deeper understanding and encounter new developments.

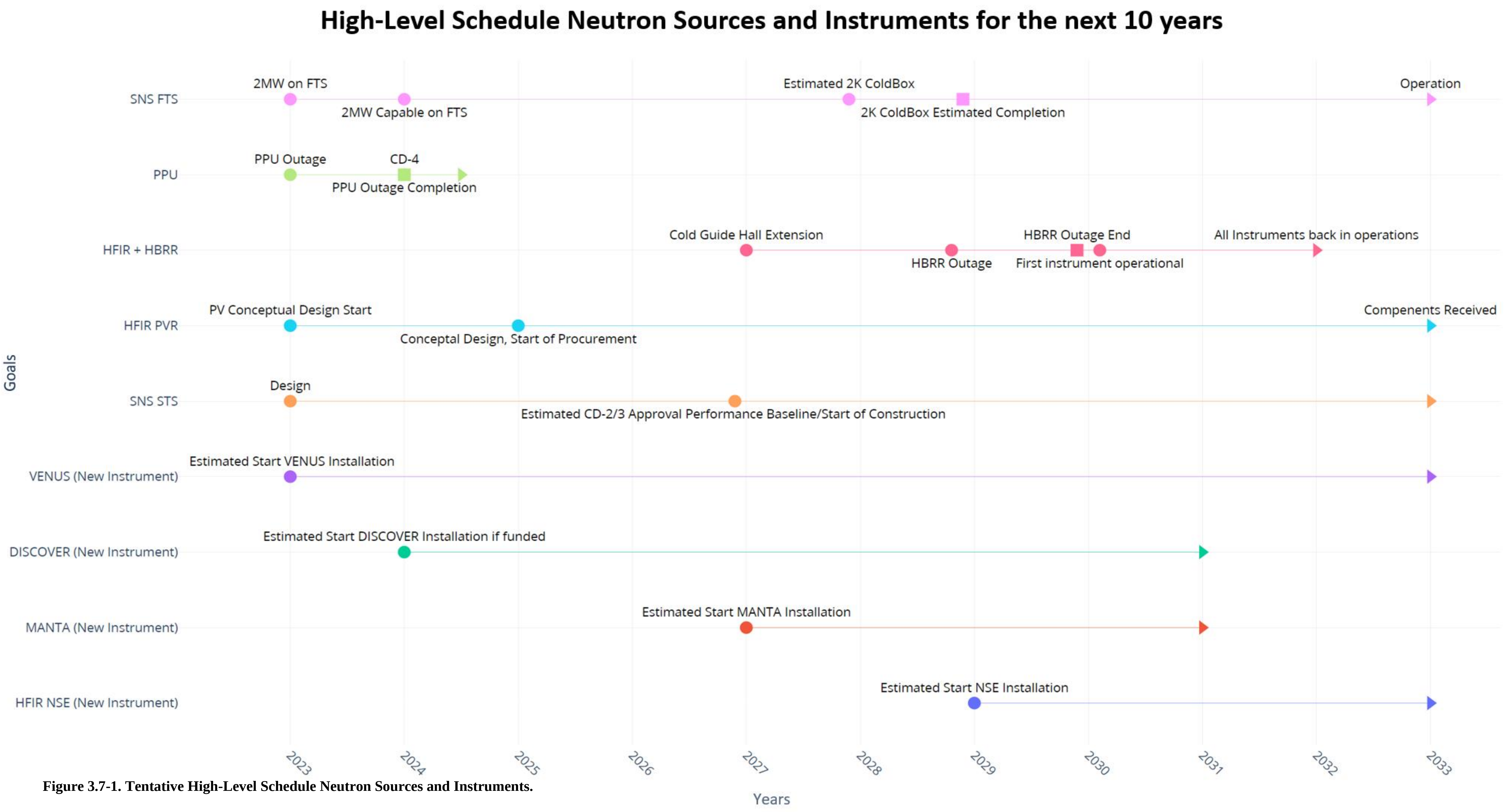


Figure 3.7-1. Tentative High-Level Schedule Neutron Sources and Instruments.

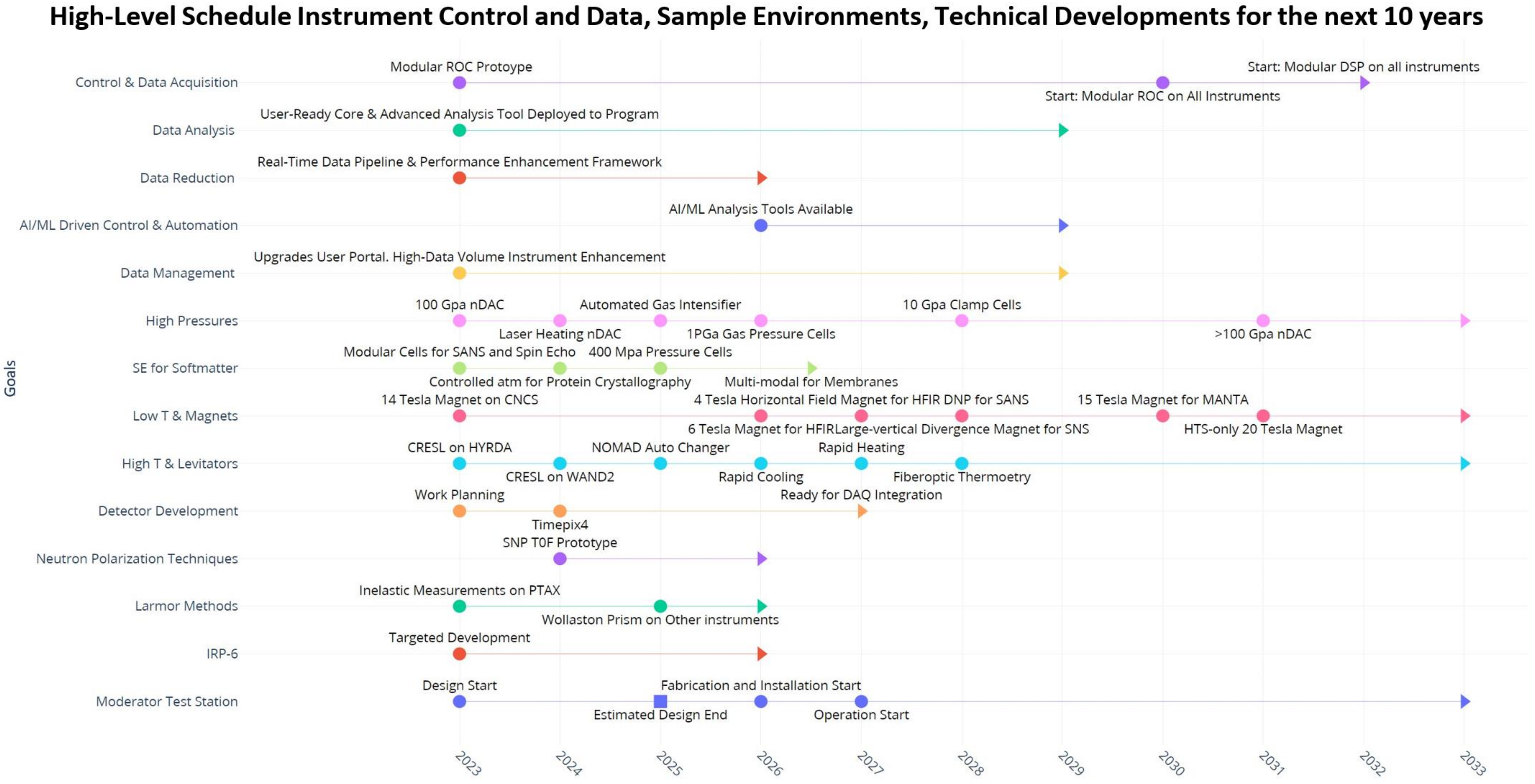


Figure 3.7-2. Tentative High-Level Schedule Instrument Control and Data, Sample Environments, Technical Developments.

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4 NON–NEUTRON SCATTERING MISSIONS

The main mission of SNS and HFIR is to run a neutron scattering program for the scientific user community. Beyond that mission, these facilities provide significant and complementary opportunities for science and societal influence. The combination of the neutron scattering program and these non–neutron scattering missions, which include radioisotope production, irradiation, fundamental physics, and accelerator physics, make NScD's facilities truly essential to DOE SC's mission and to the nation.

Historically, HFIR was designed and built to produce heavy isotopes for research in the United States. But even before HFIR started operations in 1966, researchers were considering new applications that could utilize the very high neutron flux provided by HFIR's compact core and the ORNL neutron scattering program, which was originally initiated at the Graphite Reactor in the 1940s and at the Oak Ridge Reactor in the 1950s. Fortunately, the reactor included design features that enabled a diverse portfolio of applications over the next half-century of operation. From 1986 until today, HFIR's primary mission shifted toward neutron scattering research using its beamlines. Today, HFIR enjoys true multimission endorsement for operation, with broad applications in four major areas beyond neutron scattering, including isotope production, materials irradiation testing, nuclear forensics, and fundamental physics.

Since the beginning of SNS operations in 2006, researchers realized that this facility could support an influential fundamental physics effort with no disruptions to the neutron scattering program. Not only was SNS uniquely positioned to perform breakthrough research for high-power accelerators, but also the development of an accelerator physics effort was essential to the future of this facility. This section provides a status update and forward-looking strategy for leveraging these important programs at HFIR and SNS.

4.1 Radioisotope Production

HFIR's design is optimized for isotope production. The configuration of the core, fuel, and experiment channels enable production of isotopes supporting medicine, industry, and science that cannot be produced elsewhere in the United States or the world.

4.1.1 Recent Isotope Activities

Most of the isotope production and research in the United States is led and managed by three organizations within DOE. The DOE Office of Nuclear Energy manages the production of nuclear space power isotopes, such as ^{238}Pu, used as a heat source in thermoelectric generators for NASA's deep space and rover missions. The DOE National Nuclear Security Administration manages isotopes related to maintaining and modernizing the US nuclear stockpile. The DOE SC Isotope Program manages all other isotopes produced at government facilities and laboratories, supporting research, medicine, and industry (Figure 4.1-1).

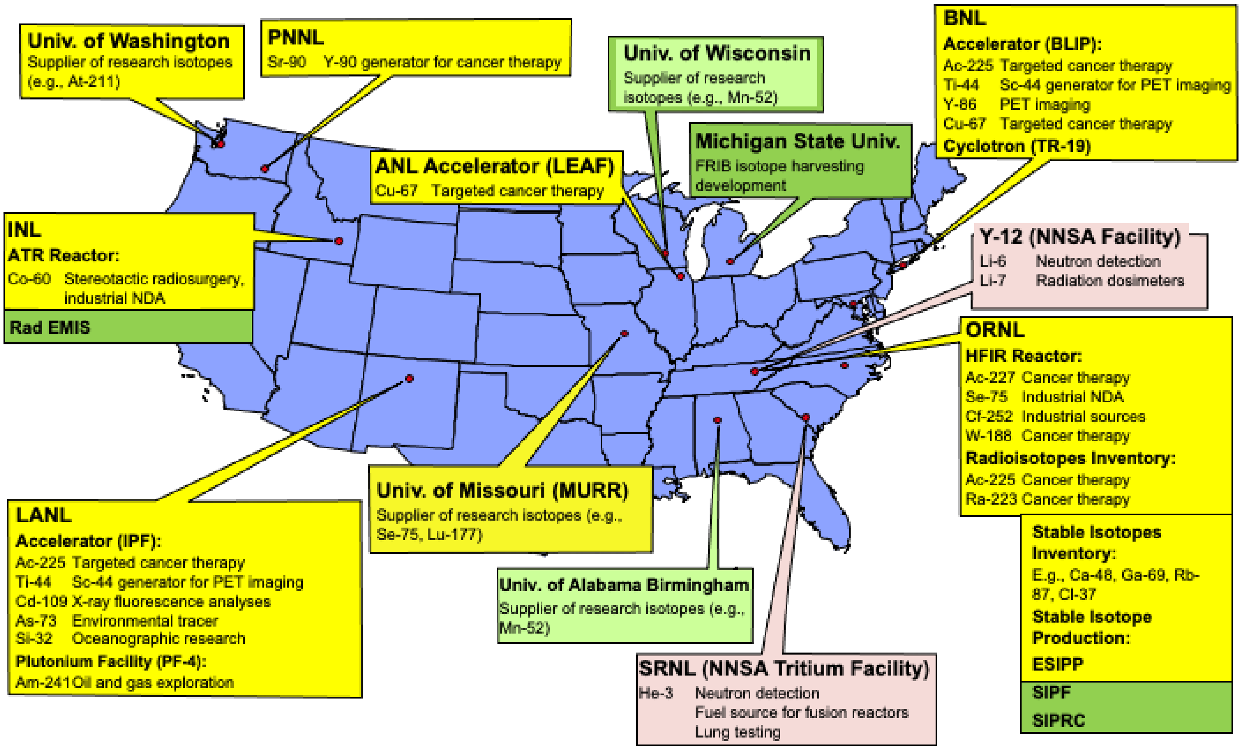

Figure 4.1-1. Production sites across the United States with example isotopes produced at each site. Credit: DOE Isotope Program managed by the DOE SC.

ORNL is the largest R&D and production site both inside and outside the DOE Isotope Program. HFIR produces the largest number of isotopes of any national facility, and because of HFIR's high thermal neutron flux, its specialty is to produce high specific activity radioisotopes as well as very heavy transplutonium isotopes that are impossible to produce in useable quantities using lower flux reactors. The only comparable reactor in the world to HFIR is the Russian SM-3 reactor in Dimitrovgrad, which has similar capabilities for isotope production but does not have neutron scattering science capability and has traditionally been operationally challenged.

In the past decade, HFIR has routinely produced many radioisotopes while also adding new isotope missions in the areas of medicine, industry, and scientific research. Medical isotope efforts now include targeted alpha- and beta-decaying therapies, which have been in the planning and trial stages for many years, but as regulatory approvals increase for these diagnostic and therapeutic isotopes, ORNL work has shifted toward a production mindset. Most notable of these therapies is the production of ^{227}Ac, which is approved by the Food and Drug Administration as a therapeutic agent marketed by Bayer Pharmaceuticals for the palliation and treatment of late-stage bone-metastasized prostate cancer. This actinium production is expected to further increase as success of this isotope grows.

HFIR continues to produce ^{75}Se for industrial radiography, often used to examine the quality of welds in the oil and gas industry. HFIR also produces ^{63}Ni continues for applications such as high-sensitivity airport personnel screening systems.

HFIR's first mission was the production of transuranium elements such as the heavy isotopes of californium, berkelium, and einsteinium, and these isotopes are still regularly produced. Transplutonium isotopes require a high thermal neutron flux, and some require longer irradiation times to transmute target materials to these heavy elements. The application of these elements covers industrial needs and fundamental research areas. For example, ^{252}Cf is used as a new reactor startup source, in mineral analyzers, and for national security purposes, whereas ^{249}Bk and other heavy isotopes are used in the discovery of super heavy elements, further expanding the periodic table as was accomplished with element 117 (Tennessine) in 2014.

4.1.2 Planned Isotope Activities

In the coming decade, continuation of the existing isotope production is anticipated, while new isotopes are also being planned with a focus on addressing new applications and reducing foreign dependence, particularly for national security and economic security applications. Although HFIR is well utilized, it is not fully utilized, and ORNL's limiting factor is hot-cell processing rather than reactor irradiation.

During the next decade, ORNL and the DOE Isotope Program will address this gap with the recently approved project to construct and operate a new state-of-the-art Radioisotope Processing Facility at ORNL. (Figure 4.1-2). This facility will offer significant additional processing capabilities from irradiation capsule opening, sorting, cleaning, and repackaging of isotope sources to significant chemical processing capabilities in modern modular hot cells and dedicated laboratory space. Additionally, this facility will support current good manufacturing processes required for medical isotope applications and will remain complementary to the existing Radiochemical Engineering Development Center, adjacent to HFIR.

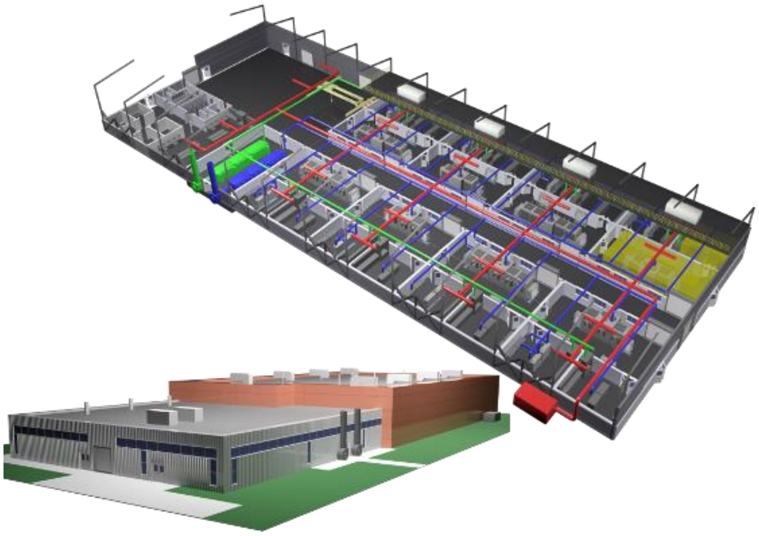

Figure 4.1-2. Future Radioisotope Processing Facility at ORNL.

Because of this upcoming capability, ORNL anticipates that irradiation needs will increase sharply after commissioning of the Radioisotope Processing Facility. Therefore, optimization of HFIR irradiation target designs, in-vessel space utilization, as well as improvements in HFIR processes and facilities will be required to match the future throughput enabled by the new hot-cell capabilities at ONRL.

Growth in medical isotopes in particular is anticipated with increased ^{227}Ac (^{223}Ra) production for Bayer's Xofigo, as well as the following new or growing medical isotope applications.

Table 4.1. New or growing medical isotope applications

Isotope	**Purpose**
^{89}Sr	Bone pain palliation
^{188}W	Cancer therapies
^{177m}Sn	Arthritis treatment in dogs
^{177}Lu	Lutathera targeted beta therapy for cancer and disease treatment

Furthermore, interest has increased in the area of isotopes used in alpha- and beta-voltaic nuclear batteries, which have applications in many industries. The need for heavy element production also continues for feeding the long-term goals of the world's heavy element research programs.

Utilization of SNS for radioisotope production is under study and evaluation. Post-PPU, SNS will be capable of delivering 2.8–3.0 MW, of which 2 MW will used by FTS. The additional power can be used for several applications, including radioisotope production.

The process to assess feasibility includes the following milestones:

- Evaluate isotopes of interest in the 1–1.3 GeV energy range
- Assess feasibility of executing the STS extraction line early in the project schedule
- Assess feasibility of utilizing SNS spent beam at the injector dump
- Create a conceptual design of an isotope production facility capable of using the SNS beam (an irradiation target station can be also added)
- Modify the SNS control systems to support beam delivery to two target stations (FTS and STS) and an isotope/irradiation production facility

In summary, isotope production was the original justification for building HFIR, and, over a half-century of operation later, it remains a critical mission and reason for continued reliable operation. Additionally, strong opportunities and interest exist for establishing feasibility of accelerator radioisotope production capabilities at SNS.

4.2 Fundamental Physics at the ORNL Neutron Facilities

4.2.1 Neutrino Physics

The neutrino is a fundamental particle at the center of some of the most compelling questions in nuclear and particle physics that have defined the frontiers of these fields for the past two decades. Since 2013, ORNL has been developing the utilization of its neutron user facilities for fundamental neutrino science. Two cutting-edge neutrino experiments, PROSPECT and COHERENT, were deployed at HFIR and SNS, respectively. Because the neutrinos are produced during normal operations, these experiments have demonstrated that these facilities can deliver world-class neutrino science while maintaining their commitments to their primary missions to the DOE BES. The COHERENT experiment at SNS has discovered coherent elastic neutrino nucleus scattering (Figure 4.2-1), and it remains the only facility where this reaction can be measured. The PROSPECT experiment has contributed significantly to the understanding of reactor neutrino experiments, and, given the unique features of HFIR, PROSPECT performs detailed studies of neutrino oscillations and searches for unknown types of neutrinos.

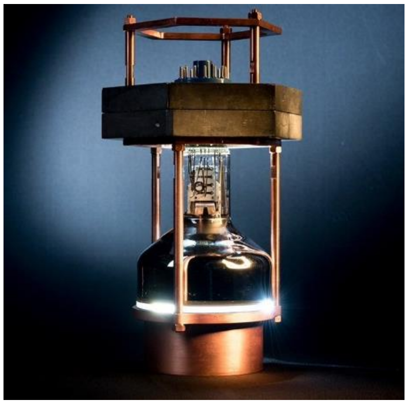

Figure 4.2-1. The world's smallest neutrino detector, a cesium iodide crystal, that discovered coherent elastic neutrino nucleus scattering at SNS.

Because neutrinos penetrate all shielding, instruments require no exclusive access to beamlines or ports. Both SNS and HFIR are planned to operate at production levels beyond the next decade with significant power upgrades in the next 5 years. A new target station planned for SNS will expand opportunities for the neutrino experimental program. A thriving collaborative experimental neutrino program is envisioned to deliver world-class science that utilizes the unique capability of these neutrino sources and is highly complementary to global neutrino experimental community efforts.

The COHERENT collaboration will deploy and operate three new instruments over the next 5 years. Future upgrades to these instruments that expand total exposure or improve resolution or signal purity will provide precision datasets that will be sensitive to new physics beyond the standard model. In the longer term, these experiments will also advance the instrumentation capability to inform a next generation set of neutrino and dark matter searches at a dedicated neutrino lab at STS, which will expand the reach of these instruments in a combination that is unrivaled in the world.

At HFIR, the success of the first PROSPECT experiment has laid the foundation for the future deployment of an upgraded instrument, PROSPECT II, that will advance the understanding of the reactor antineutrino spectrum and probe deeper searches for hidden sector particles. The compact geometry and ^{235}U composition of the HFIR core provides a unique capability to obtain the most precise measurement of the neutrino emission spectrum to resolve anomalous observations by international experiments primarily at commercial reactors in which uranium and plutonium fissions both contribute to the neutrino emissions. At an upgraded HFIR, extended runs of a larger PROSPECT-style detector could be performed that would provide unprecedented studies of reactor neutrinos and allow deep probes of the origin of dark matter in the preferred parameter space of existing models.

At SNS, PPU will increase the proton power on target from 1.4 to 2.8 MW by 2028, including an increase in neutrino production by about 50%. The beam energy will also increase by 30%, from 0.97 to 1.3 GeV. Changes to the neutrino spectrum from these energy upgrades will be sub-percent, so the primary effect is a valuable increase in the neutrino intensity while preserving all the advantages of pulsed timing for background rejection and the clear time separation of the neutrino flavor structure.

STS offers the possibility of providing the infrastructure for future neutrino detectors, including a dedicated basement experimental hallway accommodating two 10 ton neutrino detectors. The most favorable location would be on the FTS-facing side of STS, about 20 m away from the STS target monolith and 120 m away from that of FTS. In this location, neutrino detectors could simultaneously measure neutrinos in the same energy range at two very different baselines, directly testing sterile-neutrino hypotheses. An additional detector station, forward of STS, would provide appealing sensitivity to accelerator-produced dark matter.

4.2.2 Neutrinos for Safeguards

The Office of Defense Nuclear Nonproliferation R&D is becoming more interested in compact readily deployable instruments for advanced reactor and spent fuel monitoring made possible by the groundbreaking work carried out at HFIR. HFIR is an attractive location to develop instrumentation and technologies for these applications. Together with safeguards practitioners, ORNL can provide a mission-focused testbed in bringing this new capability to maturity.

4.2.3 Fundamental Neutron Symmetries

The neutron is a critical tool in fundamental physics, used to address some of the most compelling science questions in nuclear and particle physics, astrophysics, and cosmology. Whereas the neutron primarily serves the neutron scattering community as a probe of other materials, the fundamental neutron physics community is interested in studying the properties of the neutron itself along with its interactions. Performing high-precision measurements of neutrons can enable the development of a more complete understanding of the four fundamental forces of nature—the electromagnetic, weak, strong, and gravitational interactions. It can also address the following basic questions about the nature of matter in the universe. Why is the universe made up of matter but virtually no antimatter? Which particles make up the mysterious dark matter in the universe? Do more fundamental underlying symmetries describe the laws of physics beyond the highly successful standard model of particle physics?

A world-leading program of fundamental neutron physics research has been developed at the Fundamental Neutron Physics Beamline (FNPB [BL-13]) at SNS. In an early success for FNPB, the hadronic weak interaction was characterized in exceptional detail by searching for parity-violating asymmetries in neutron interactions. The $n + p \geq d + \gamma$ process was studied, and for the first time the weak interaction between the neutron and the proton was measured. Subsequently, the world's first parity-violating asymmetry in the neutron–^{3}He weak interaction was measured. In the coming years, the Neutron "a" "b" experiment, now commissioning at FNPB, and a future version using polarized neutrons, will measure key weak interaction parameters with unprecedented precision to shed light on a puzzle in nuclear beta decay that might be a sign of new physics. Additionally, as part of a new program of research on novel dark matter candidates, a recent search for neutrons disappearing into dark mirror neutrons has ruled out an exotic explanation for the neutron lifetime anomaly, a long-standing discrepancy between different techniques to measure the neutron decay lifetime. This new program will also provide important R&D opportunities for future high-sensitivity searches for neutrons transitioning into antineutrons. Matter transforming directly into antimatter has never been experimentally observed and would have immediate implications for the observed matter-antimatter asymmetry in the universe.

Another critical ingredient to explain the lack of antimatter in the universe is the violation of a fundamental symmetry, which is linked to another property of the neutron. The neutron might have an electric dipole moment (nEDM), which would describe how electric charge might be asymmetrically distributed inside the overall neutral particle. From its origins at the ORNL Graphite Reactor to today, the search for the nEDM has eliminated numerous proposed theories and extensions to the standard model and remains one of the most compelling experimental pursuits in nuclear physics (Figure 4.2-2). The next decade will see the installation and commissioning of the world's most ambitious search for the nEDM at the FNPB at the SNS. The nEDM@SNS experiment uses a unique approach in which the cold neutron beam from the FNPB is used to create ultracold neutrons—which have such low energy that they are totally internally reflected in material bottles—and trap them within the experiment cell. This experiment will improve the current limit on the nEDM by almost two orders of magnitude and is the highest priority for the fundamental neutron physics community.

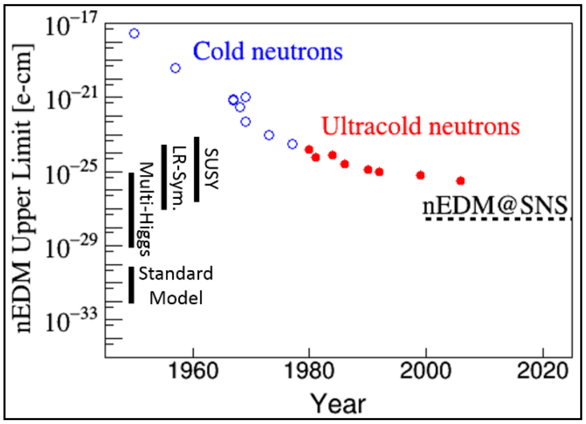

Figure 4.2-2. History of limits from neutron electric dipole moment (nEDM) searches using cold and ultracold neutrons, and the projected limit from the nEDM@SNS experiment. Predictions from the standard model and some theoretical extensions are shown along the vertical axis.

Peering beyond the next decade, continuing to push the frontiers of human knowledge will require not only advances in experimental technology but also substantial increases in neutron intensity available for experiments. Fundamental physics applications benefit most from colder neutrons thanks to higher cross sections, longer residence time in the experiment, and lower systematic corrections. Next-generation neutron experiments that tackle these physics questions will require the highest flux and lowest velocity neutrons possible to achieve their sensitivity goals. A future high-impact fundamental neutron physics program would be possible at the SNS STS. Furthermore, because fundamental neutron physics experiments are primarily concerned with high time-averaged intensity, a cold beamline at HFIR would be especially exciting for the community. The planned upgrade of the HFIR pressure vessel creates an interesting possibility. By including considerations in the design of the new pressure vessel, the development of a competitive source of ultracold neutrons becomes possible. Such a facility would give rise to a new and diverse class of experiments at ORNL. These upgraded facilities represent excellent opportunities to build on the success at SNS's FNPB and to continue a world-leading fundamental physics program at ORNL.

4.2.4 Muonium

Precision studies of muonium, the bound state of a positively charged muon and a negatively charged electron, provide an exceptionally clean system to study beyond the standard-model physics in the lepton sector. The proposed Single-Events Effects and Muon Spectroscopy (SEEMS) facility at SNS (Section 4.4) with a muon flux of approximately 6.8×10^9 μ^+/s would provide a world-leading facility for precision studies of the muon with a muon flux that can exceed current facilities by two orders of magnitude. Phenomena like lepton flavor violation has been observed in neutral particles through processes like neutrino oscillations, yet it has not been seen in the transitions of charged leptons, such as e, m, and t. The SEEMS facility at SNS would become a world-leading location to execute a program to study charged lepton flavor violation, which is a field that is actively being studied around the world. Observation of lepton flavor violation processes such as $\mu \rightarrow e\gamma$, $\mu \rightarrow eee$ would immediately confirm the presence of new interactions, beyond the currently known ones, that address some of the most fundamental questions in particle physics. The process of muonium oscillations, $\mu^+ e^- \rightarrow \mu^- e^+$, that can be uniquely probed at SEEMS, along with the processes mentioned earlier, will put constraints on the scale of the new physics. Precision measurements of the muon's fundamental properties, such as the magnetic moment and the electric dipole moment (EDM), will also inform the scale and nature of the new physics.

Studies of the level spectra of muonium, in particular its hyperfine structure, can also provide the most sensitive tool for testing quantum electrodynamics and even discover possible new interactions affecting the atomic properties. For example, it can help answer whether the puzzle of the proton radius can be resolved by possible new physics contributions. The proton radius puzzle relates to the size of the proton. Historically the proton charge radius was measured by two independent methods that converged to a value of about 0.877 fm. This value was challenged using the third method, using muonic hydrogen, which produced a different radius by five standard deviations. In muonic hydrogen, the electron is replaced by a negatively charged muon. Muonic hydrogen atoms are much smaller than typical hydrogen atoms because the much larger mass of the muon gives it a much more localized ground-state wavefunction than is observed for the electron. Muonium eliminates the uncertainties associated with the strong interactions of the proton and can help answer the proton radius puzzle.

4.2.5 Nuclear Structure and Spectroscopy

A sustained and enhanced neutron science program at HFIR is possible by deploying state-of-the-art detector technology that is capable of complete, correlated spectroscopy that is ultrasensitive to weak radiation signatures. A future HFIR Decay Station (Figure 4.2-3) on a neutron beamline and rabbit system, in combination with an Online Isotope Facility, would make ORNL a unique world center for both basic and applied nuclear physics, enabling several crosscutting missions and inquiries, including the following:

- Correlation of triaxial deformation of n-rich nuclei with inertial dynamics, masses, moments, charge radii, and r-process nucleosynthesis
- Search for cross-shell excitations, single-particle fragmentation, and shape coexistence of n-rich nuclei near or beyond double-magic ^{132}Sn and ^{78}Ni
- Quantification of nucleon–nucleon correlations and the role of the p–n interaction in driving nuclear deformation
- Investigation of beta, gamma, and neutron spectra shapes of n-rich nuclei for decay heat/reactor design, fundamental science, and nuclear forensics
- Investigation of interface between nuclear, atomic, and molecular spectroscopy using traps and lasers for fission dynamics, EDM searches, and ground-state properties of exotic nuclei
- Investigation of fission electron yield integrals for reactor neutrino anomaly
- Ultrasensitive material identification, radiation localization (imaging), and quantification for forensics and detection science
- Investigation of transmutation vs. burnup cross sections of actinides and β-delayed neutrons
- Correlation of event-by-event fission dynamics

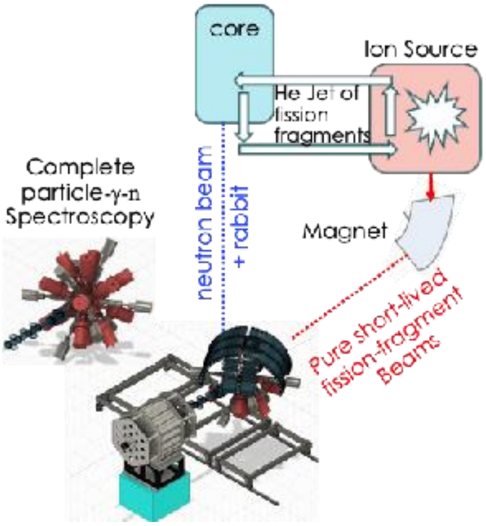

Figure 4.2-3. Schematic view of the future HFIR Decay Station and Online Isotope Facility for basic and applied sciences.

4.3 Accelerator Science and Technology Research

Accelerator science and technology research motivates the development of accelerators and is an essential component of any accelerator-based facility. As the world's highest power proton accelerator and the world's highest energy proton linac, SNS is uniquely positioned to perform breakthrough research for high-power accelerators. The accelerator research portfolio is centered on high-impact projects that require beam parameters and accelerator infrastructure currently only found at SNS.

DOE vigorously supports accelerator R&D through focused programs in basic energy sciences, high-energy physics, and nuclear physics and through the Accelerator Research and Development and Applications that provides coordination within the DOE SC. In a 2021 report, investment in NScD's advanced research facilities was identified as one of the critical areas in which to match the significant investment planned in the international landscape. Many strong returns are possible for a facility on the investment in accelerator science and technology. For the short-to-medium term (approximately 1 to 5 years), the investment improves the facility's present capability and performance, it fosters science productivity and visibility in the community through publications and invited talks, and it attracts and retains talented staff and creates opportunities for external funding. SNS has an excellent track record in acquiring and leveraging DOE and National Science Foundation funding in accelerator science and technology. For the medium-to-long term (approximately 5 to 10+ years), the investment in accelerator science and technology ensures facility mission readiness by enabling future opportunities.

From the beginning of SNS operations in 2006, the strategy has consistently been to leverage the staff core competencies in accelerator R&D by tailoring a program that is focused on specific high-impact research in high-intensity beams, superconducting radio frequency (SRF) technology, and high-power technology. Plasma processing and 6D measurement of the beam phase space are examples of novel techniques developed and demonstrated at SNS.

The overarching long-term goal of SNS accelerator science and technology is to enable high-power beams and the realization of hadron facilities in the multi-megawatt power regime. Multi-megawatt power offers unlimited potential in developing facilities, including high-power neutron sources, and in supporting medical and industrial applications (i.e., accelerator-driven systems, irradiation facilities).

Figure 4.3-1 presents a 10 year roadmap of accelerator science and technology research that leverages and develops NScD's present capabilities toward the demonstration of multi-megawatt facilities.

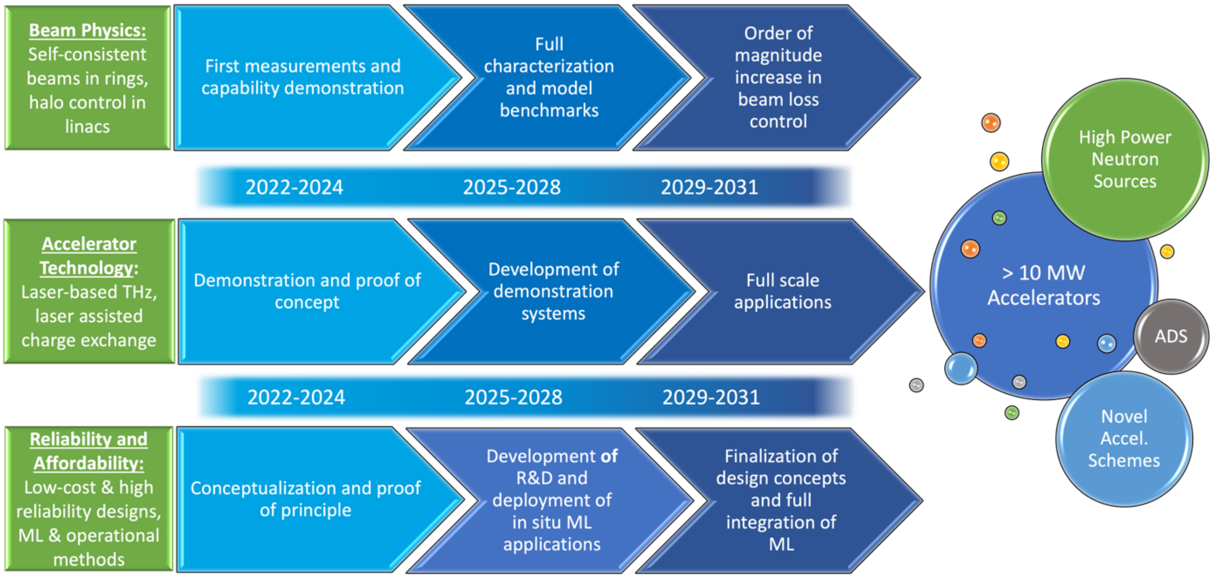

Figure 4.3-1. 10 year roadmap of accelerator science and technology research.

The Accelerator Science and Technology Research program uses unique facility capabilities to make progress in several key areas that will advance the frontier of high-intensity machines and will also contribute broadly to other areas of accelerator science. Research efforts can be categorized into three main themes: (1) beam physics for high-intensity accelerators, (2) advancements in key accelerator technologies, and (3) improvements in accelerator affordability and reliability. Although the research portfolio is quite extensive, for the sake of brevity, only the highest impact projects are highlighted here.

4.3.1 Beam Physics

The beam physics research program is centered primarily on controlling collective effects in high-intensity beams. The ultimate goal is to improve beam loss by at least an order of magnitude to enable the next decade of high-intensity facilities.

4.3.1.1 Self-Consistent Beams

A beam halo is generated in accumulator rings primarily by the beam's nonlinear space charge force. High-intensity beams are typically injection painted in the ring, allowing some freedom in the beam's density distribution. One special form of beam distributions is the self-consistent distribution, which consists of uniform ellipses in real space that yield linear space charge forces inside the beam, thus avoiding the nonlinearity issues. A self-consistent beam in an ideal linear lattice should not generate any beam halo and should maintain uniform density independent of beam intensity. As a result of these attractive properties, self-consistent beam distributions have been heavily utilized in analytical and computational studies of beam physics, especially for exploring resonance behavior in rings. However, they have not yet been realized in practice in an accumulator ring. The main challenge has been maintaining the self-consistency during the intensity accumulation process. A subclass of these distributions, called rotating distributions, that can be realistically injection painted while maintaining the self-consistency requirement was theoretically proposed by V. Danilov [1] shortly after the SNS facility was constructed.

This project aims to experimentally demonstrate injection-painted self-consistent beams of the form proposed by Danilov in the SNS ring and to explore their properties experimentally, including their intensity dependence and response to resonance conditions. The long-term goal is to understand whether self-consistent beams can be used to mitigate space charge effects at next-level beam intensities.

- Milestone 1: Achieve fully self-consistent injection painted beams (2023)
- Milestone 2: Explore characteristics of self-consistent beams (2026)
- Milestone 3: Create 10 MW ring design utilizing self-consistent beams (2030)

4.3.1.2 Control of Space Charge in Linear Accelerators

At present, the most successful strategies for beam loss control in linacs are largely heuristic, relying on operator intuition rather than predictive models. Despite decades of improvements, models cannot accurately predict the evolution of the beam distribution, particularly the very outer edges of the beam referred to as the beam halo. The problem is thought to lie in a few historical knowledge and capability gaps: most importantly, the lack of an experimentally measured 6D initial phase space distribution of the beam at the start of the linac, and the capability to measure the beam phase space at the one part per million level required to characterize beam halo. These two key capabilities have recently been demonstrated for the first time at the Beam Test Facility, enabling a promising research initiative aimed at characterization, modeling, and control of beam halo driven by space charge, a leading source of beam loss in linacs. The work will be conducted at the Beam Test Facility, but new methods and knowledge gained will be implemented and validated on the SNS production accelerator.

- Milestone 1: Measure and characterize beam halo (2023)
- Milestone 2: Obtain model agreement to the level of beam halo (2026)
- Milestone 3: Develop and implement methods for control and removal of beam halo (2029)

4.3.2 Accelerator Technology

In the area of accelerator technologies, breakthrough research areas leverage unique capabilities and facilities at SNS. The following projects will have widespread significance for the accelerator community.

4.3.2.1 Laser-Assisted Charge Exchange Injection

Short-pulse high-power hadron accelerators rely on charge-exchange injection to convert an H^- pulse from a linac into a proton pulse. In the conventional implementation of this scheme, a micrometer-thin carbon foil is used to strip the electrons from the H^- after merging with the circulating proton beam at the injection point to the ring. The foil technology has two major limitations: (1) it produces locally high levels of beam loss and residual activation from particle scattering, and (2) the foils sublimate beyond a threshold power density level, recently identified to be below 10 MW for SNS and similar schemes.

Laser-assisted charge exchange (LACE) is a novel, material-free method of H^- charge exchange that has been under development at SNS for the last decade and does not suffer from these limitations. In this method, the foil is replaced by two magnets and a laser. H^- beam energies on the order of at least 1 GeV are required, making SNS uniquely capable of developing this technology. The main challenge is the high average laser power needed for a full duty cycle application. Thus far, high-efficiency LACE has been demonstrated at SNS for H^- beams up to microseconds in duration. It remains to scale this technology to millisecond-long pulses at high repetition rates with conventionally available lasers and to demonstrate injection of the stripped particle into the ring. A new scheme called sequential resonance excitation, which uses the laser to excite the inner electron to the $n \geq 3$ quantum state in a stepwise fashion, has the potential to overcome the historical power hurdle even for conventional laser technology. The goal of this program is the experimental validation of the sequential resonance excitation method and the demonstration of a laser charge exchange test system in the SNS ring injection region. Upon successful completion of this project, new high-power ring design concepts, which are absent of the usual constraints imposed by the stripper foil, will be evaluated.

- Milestone 1: Validate experimental sequential resonance excitation scheme (2023)
- Milestone 2: Develop LACE injection demonstration system (2027)
- Milestone 3: Design 10 MW ring with LACE injection system (2031)

4.3.2.2 Laser-Based Terahertz Generation

The goal of this research program is to pursue innovative concepts and research topics relevant to state-of-the-art and future accelerators using a tabletop intense laser platform. A new research initiative using a tabletop terawatt-class laser at infrared wavelengths has started in the Research Accelerator Division. The infrastructure uses an ultrafast multi-millijoule titanium–sapphire drive laser to generate intense terahertz radiation via optical rectification in organic crystals. The tabletop laser system aims at achieving field strength up to 1 GV/m at 1 kHz repetition rate. Intense fields available with this laser system will enable research toward innovative particle acceleration concepts as well as concomitant research topics related to field emission or probing of normal conducting and superconducting materials. The new R&D initiative is first focusing on the generation and characterization of intense beams at near-infrared, mid-infrared, and terahertz wavelengths by using optical parametric amplification and optical rectification.

- Milestone 1: Ramp up terahertz intensity and field emission scanner (2023)
- Milestone 2: Develop ion acceleration concept using terahertz radiation (2024)
- Milestone 3: Accelerate ions in experimental demonstration using terahertz radiation(2028)

4.3.3 Reliability and Affordability

A significant portion of the research portfolio at SNS is centered on improving the reliability of the facility, now at around 90%, and improving the affordability of a future facility at SNS.

4.3.3.1 Low-Cost Accelerator Designs

As accelerators continue to increase beam energy, power, and luminosity, improving the cost-effectiveness of designs is important. In this research thrust, compact, cost-effective designs will be developed both for proton SRF facilities and for x-ray free electron laser (FEL) sources.

The goal of the proton SRF project is to develop a design in which all SRF cavities fully utilize the available radio frequency power. Each section will be optimized by maximizing its cavity voltage and letting the beam pass through the same cavities several times until the combined current approaches the technical limit. Compared with a single-pass scenario, the number of cavities in each section is reduced inversely proportionally to the number of passes, or recirculations, thus making the accelerator more compact. The results of the proposed work will be applicable to a broad range of future high-power accelerators of any purpose.

The compact x-ray FEL project will focus on the development of an energy-recovery linac (ERL)-based compact x-ray FEL. This concept has three significant advantages compared with traditional single-pass x-ray FELs: (1) recirculating SRF linac makes the accelerator facility compact, (2) energy recovery in the SRF linac saves the klystron power and reduces the beam dump power, (3) the high average beam power produces a high average photon brightness. Design of such an ERL to achieve the desired beam qualities is extraordinarily challenging; however, if successful, it will provide an opportunity to have a compact, cost effective, and high performing photon source to complement the existing neutron source for materials science.

These two projects will proceed along similar trajectories:

- Milestone 1: Initial concept exploration and identification of key design elements (2023)
- Milestone 2: High-fidelity simulations of designs, identification of technological gaps (2026)
- Milestone 3: Technical design report for a future facility (2031)

4.3.3.2 High-reliability accelerator technologies

R&D in this area is aimed at developing advanced accelerator concepts for the next-generation high-power SRF proton linacs, enabling their applications for societal benefits such as accelerator-driven system (ADS) and medical treatment. The accelerator requirements in machine reliability and availability for these applications are much more stringent. Achieving them, especially for ADS-class high-power (10–20 MW) proton linacs, is an outstanding challenge.

The current R&D plan is (1) to develop a reliability/availability model including beam trip and recovery based on the actual operation data of the SNS accelerator and to identify areas for improvement that require new technologies and (2) to develop new concepts for highly reliable SRF systems and to suggest directions for future development activities. The outcome of the R&D will lead to an opportunity for a short-demonstration SRF system, enabling advanced SRF proton accelerators for societal applications in transformative cancer treatment as well as in ADS-based nuclear waste reduction, and perhaps even nuclear electricity generation.

- Milestone 1: Develop a reliability/availability model (2022)
- Milestone 2: Develop a concept for a highly reliable accelerator including subsystems (2023)
- Milestone 3: Develop a demonstration SRF system (2028)

4.3.3.3 Machine Learning and Operational Methods for Improved Reliability

The goal of this project is to extend and integrate ML techniques in a robust framework to enable timely and reliable condition monitoring, failure prediction, and parameter optimization of accelerator equipment. The current approach to maximizing availability of the SNS accelerator and target includes monitoring and thresholding subsystem performance, regular and pre-emptive equipment maintenance, and continuous optimization of designs. Unfortunately, this approach does not take full advantage of the vast quantities of self-monitoring data available from the facility. ML methods can digest and analyze data on scales exponentially larger than human capability and thus provide a tremendous opportunity to revolutionize the approach to ensuring machine availability. The ML methodology in this project focuses on time-series analysis for anomaly detection, classification and prediction, and surrogate modeling for performance optimization of equipment subsystems that would otherwise require unrealistically heavy computational loads. Success in this project will improve availability at user facilities by (1) providing early warning of performance degradation or failure of equipment, (2) allowing smarter maintenance decisions and cost-effective asset management, and (3) introducing a powerful methodology for optimizing and designing equipment for longer lifetimes.

- Milestone 1: Demonstrate ML capabilities in four strategic areas: beam signals, high-voltage converter modulator, targets, and cryogenic moderator system (2024)
- Milestone 2: Complete first fully operational ML systems for three use cases; use ML for target design (2027)
- Milestone 3: Develop ML as an integrated tool throughout the accelerator (2030)

4.4 Single-Event Effects and Muon Spectroscopy Facility

The SEEMS facility is planned to be a small-scale version of a target station at SNS. Containing a solid tungsten target and six beamlines, this user facility will simultaneously serve two distinct communities with world-leading capabilities for each.

The first community exploits high-resolution muon spectroscopy (μSR) techniques. Despite a history of pioneering developments of the μSR technique in the United States, no facility in the United States is capable of performing these experiments. The SEEMS research facility would fill this lack of domestic scientific capability, and it would represent an orders-of-magnitude increase in flux over any pulsed μSR source currently in operation. A basic research technique, μSR is highly complementary to neutron scattering, serving research in quantum materials, radical chemistry, engineering, and battery materials. In this way, it extends the three-source strategy by adding a fourth source that focuses on the same scientific questions, providing complementary data and strengthening the scientific impact of the ORNL user program.

The second user community served by SEEMS is research and testing of electronics for vulnerabilities to cosmogenic radiation (i.e., single-event effects [SEE]). These phenomena are an urgently growing concern to commercial aviation, ground transportation, autonomous ground and air transportation, high-integrity computing, spacecraft, and defense applications. SEEMS will provide varied radiation conditions for rapid testing and evaluation of small electronic devices and large complete systems. SEEMS will provide four times more test time compared with one existing facility, while adding capabilities. This capability adds to the industrial and scientific use of neutrons at ORNL and is another important use of the SNS accelerator.

The technology of the SEEMS target station at SNS can simultaneously serve both the μSR and SEE missions—without affecting the primary neutron scattering science target station(s). Only 0.2% of the SNS accelerator beam will be sent to the SEEMS target station. With the relative youth and high availability of the SNS accelerator, the SEEMS facility will operate for 4,500 h annually and for decades to come. The strength of this concept was noted at several workshops:

- At the 2014 Quantum Condensed Matter Grand Challenge workshop in Berkeley, California, where the participants concluded, "It should be considered whether it makes sense to build a muon facility collocated with SNS."
- At a 2016 workshop at ORNL in response to this urging, a panel of worldwide μSR experts noted, "… the most exciting conclusion from the meeting was the entirely unanticipated development of a novel source design at the SNS… with strong encouragement from all involved that this source design be developed."
- In 2019, a committee of SEE researchers from academia and the aerospace industry met and summarized, "The aerospace/avionics perspective is that the need for a US test facility like SEEMS is urgent."
- In 2021, a follow-on workshop to understand the scientific impact of a μSR source like SEEMS in the United States concluded, "…this would be an excellent opportunity to develop a US-based μSR facility and would be best positioned to develop new low-energy μSR beams that can push the capabilities [of μSR]."

The facility concept has the potential to be a world-leading facility in both of its designed missions. First, by utilizing the existing accelerator at SNS, it is possible to power a pulsed μSR facility that would have the highest flux and best time resolution compared with any currently existing μSR source. Second, this high-throughput platform would perform neutron irradiation of electronic devices and systems for SEE testing, far exceeding capabilities at any facility worldwide. Key to the design is pioneering work performed at ORNL in developing laser stripping technology that makes possible the short, intense proton pulse necessary for this facility, with insignificant effect on the neutron scattering science mission of SNS. Furthermore, the existing resources at ORNL and SNS provide the means to construct this facility for a fraction of the cost of a new dedicated accelerator facility, in a much shorter timescale, and with lower operational costs by taking advantage of the existing user facilities.

The current concept of the SEEMS facility (Figure 4.4-1) relies on using laser stripping to extract a proton pulse just before the injection ring. The proton pulse would be 30 ns and 50 kHz, which are optimized for muon production while maintaining good resolution. The target would be a solid tungsten target, and thus capable of producing both high-energy neutrons for SEE testing and pions for μSR. The design includes two identical testing stations receiving high-energy neutron beams at the ±30° beamline positions. These stations are each 9 m × 3 m (interior area) testing stations offering two irradiation positions: one for device testing and one for system testing. Additionally, four beamlines would be available for μSR, two on each side of the target utilizing muons ejected at ±90° from the proton beam. This configuration reduces background from other particles produced in the target, and the high flux would be capable of supporting conventional surface muon beams and low-energy μSR experiments, which are in high demand in the community. Additional space would be available downstream from the target for future expansion.

Currently, the concept is not funded, funding to complete the conceptual design is being sought. An estimated 2 years are needed to complete the conceptual design, and a further 8 years to construct the facility and begin user operations. When complete, it could run whenever the SNS accelerator is operational and could be integrated into the user program as a separate user facility at ORNL.

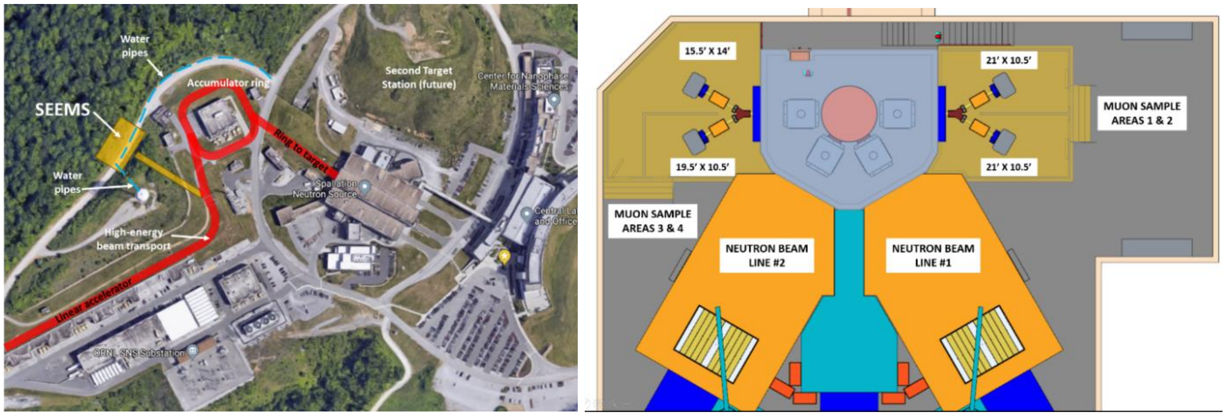

Figure 4.4-1. Proposed location of the SEEMS facility and beamline locations. (left) The proposed location for the SEEMS facility, northwest of the linac and accumulator ring. This location would provide the shortest path for the protons, which will be extracted just before the accumulator ring. (right) The proposed locations of the beamlines (not to scale). Two SEE test caves would be located at the ±30° positions, and two μSR beamlines would be positioned on each side of the target, taking beam from the ±90° directions.

REFERENCES

[1] V. Danilov, S. Cousineau, J. Holmes, S. Henderson, “Self-Consistent Time Dependent Two Dimensional and Three Dimensional Space Charge Distributions with Linear Force,” Phys. Rev. ST Accel. Beams 6 (2003): 094202. https://doi.org/10.1103/PhysRevSTAB.6.094202.

APPENDIX A. ABBREVIATIONS

μSR	muon spin rotation/relaxation/resonance
ADARA	Accelerating Data Acquisition, Reduction, and Analysis
ADS	accelerator-driven system
AI	artificial intelligence
BER	Biological and Environmental Research
BES	Basic Energy Sciences
BESAC	Basic Energy Sciences Advisory Committee
CD-1	Critical Decision 1
CNMS	Center for Nanophase Materials Science
COVID-19	coronavirus disease 2019
CSMB	Center for Structural and Molecular Biology
DFT	density functional theory
DMFT	dynamical mean field theory
DMRG	Density Matrix Renormalization Group
DNP	dynamic nuclear polarization
DOE	US Department of Energy
DOI	digital object identifier
EERE	Energy Efficiency and Renewable Energy
EDM	electric dipole moment
EES	electrical energy storage
ERL	energy-recovery linac
ESH&Q	Environment Safety, Health, and Quality
FAIR	findable, accessible, interoperable, and reusable
FEL	free electron laser
FLOSS	Free/Libre Open-Source Software
FNPB	Fundamental Neutron Physics Beamline
FTS	First Target Station
FWHM	full-width-at-half-maximum
HBRR	HFIR Beryllium Reflector Replacement
HFIR	High Flux Isotope Reactor
HPC	high-performance computing
HTS	high-temperature superconductor
HYSPEC	Hybrid Spectrometer
ICEMAN	Integrated Computational Environment for Modeling and Analysis
IRP	inner reflector plug
J-PARC	Japan Proton Accelerator Research Complex
LACE	laser-assisted charge exchange
LTS	low-temperature superconductor

MD	molecular dynamics
ML	machine learning
MTS	Moderator Test Station
NAS	National Academy of Sciences
nEDM	neutron electric dipole moment
NN	neural network
NOMAD	Nanoscale Ordered Materials Diffractometer
NP	Office of Nuclear Physics
NScD	Neutron Sciences Directorate
ORNL	Oak Ridge National Laboratory
PEI	polyethylenimine
PEO	polyethylene oxide
PPU	Proton Power Upgrade
PVR	Pressure Vessel Replacement
QENS	quasi-elastic neutron scattering
QMC	quantum Monte Carlo
qubits	quantum bits
SANS	small-angle neutron scattering
SC	Office of Science
SEE	single-event effect
SEEMS	Single Events Effects and Muon Spectroscopy
SMS	Streaming-Message-Server
SNP	spherical neutron polarimetry
SNS	Spallation Neutron Source
SRF	superconducting radio frequency
STS	Second Target Station
TOF	time-of-flight

APPENDIX B. INSTRUMENT NAMES AND LOCATIONS

Shortened name	Instrument name	Facility	Location
ARCS	Wide Angular-Range Chopper Spectrometer	SNS	BL-18
BASIS	Backscattering Spectrometer	SNS	BL-2
BIO-SANS	Biological Small-Angle Neutron Scattering Instrument	HFIR	CG-3
CNCS	Cold Neutron Chopper Spectrometer	SNS	BL-5
CORELLI	Elastic Diffuse Scattering Spectrometer	SNS	BL-9
CTAX	Cold Neutron Triple-Axis Spectrometer	HFIR	CG-4C
DEMAND	Dimensional Extreme Magnetic Neutron Diffractometer	HFIR	HB-3A
DISCOVER	Diffractometer for Materials Discovery	SNS	NEW
EQ-SANS	Extended *Q*-Range Small-Angle Neutron Scattering Diffractometer	SNS	BL-6
VERITAS	Versatile Intense Triple-Axis Spectrometer	HFIR	HB-1A
FNPB	Fundamental Nuclear Physics Beam Line	SNS	BL-13
GP-SANS	General-Purpose Small-Angle Neutron Scattering	HFIR	CG-2
HIDRA	High Intensity Diffractometer for Residual stress Analysis	HFIR	HB-2B
HYSPEC	Hybrid Spectrometer	SNS	BL-14B
IMAGINE	Laue Diffractometer	HFIR	CG-4D
LIQREF	Liquids Reflectometer	SNS	BL-4B
MANDI	Macromolecular Neutron Diffractometer	SNS	BL-11B
MAGREF	Magnetism Reflectometer	SNS	BL-4A
MANTA	Multi-ANalyzer Triple-Axis Spectrometer	HFIR	NEW
MARS	Multimodal Advanced Radiography Station	HFIR	CG-1D
NOMAD	Nanoscale-Ordered Materials Diffractometer	SNS	BL-1B
NSE	Neutron Spin Echo Spectrometer	SNS	BL-15
HFIR NSE	Neutron Spin Echo at HFIR	HFIR	NEW
POWDER	Neutron Powder Diffractometer	HFIR	HB-2A
POWGEN	Powder Diffractometer	SNS	BL-11A
PTAX/HB-1	Polarized Triple-Axis Spectrometer	HFIR	HB-1
SEQUOIA	Fine-Resolution Fermi Chopper Spectrometer	SNS	BL-17
SNAP	Spallation Neutrons and Pressure Diffractometer	SNS	BL-3
TAX/HB-3	Triple-Axis Spectrometer	HFIR	HB-3
TOPAZ	Single-Crystal Diffractometer	SNS	BL-12
USANS	Ultra-Small-Angle Neutron Scattering Instrument	SNS	BL-1A
VENUS	Versatile Neutron Imaging Instrument at the SNS	SNS	NEW
VISION	Vibrational Spectrometer	SNS	BL-16B
VULCAN	Engineering Materials Diffractometer	SNS	BL-7
WAND^2	Wide-Angle Neutron Diffractometer	HFIR	HB-2C