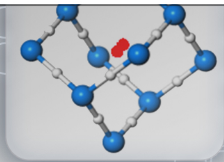

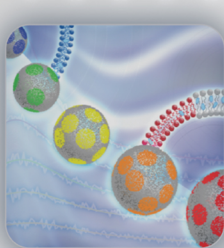

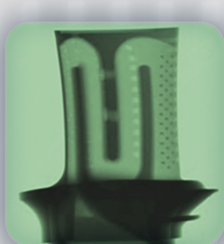

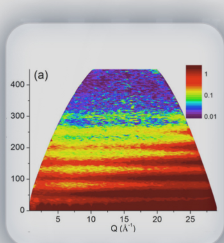

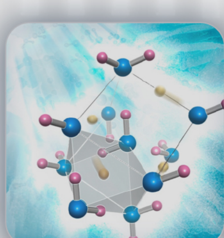

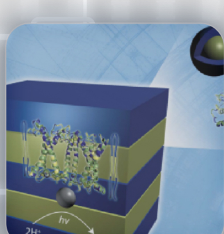

Oak Ridge National Laboratory

Neutron Sciences

Spallation Neutron Source • High Flux Isotope Reactor

Strategic Plan 2014

EXECUTIVE SUMMARY AND DIRECTOR'S MESSAGE

Executive Summary

Neutron scattering is a key technique for advancing the science and technology of materials important in biology, chemistry, physics, and engineering. The uniqueness of the neutron as a probe for 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) at Oak Ridge National Laboratory (ORNL) enables the research carried out by the scientific community by providing a powerful array of neutron capabilities for our users.

The strategic plan presented here ensures that ORNL will continue to provide the neutron facilities required to address existing and future major energy challenges and to ensure that the United States maintains a forefront position in future research utilizing neutrons. The plan identifies four science priorities where neutrons are a crucial tool for characterizing structure and dynamics: quantum materials, materials synthesis and performance, soft molecular matter, and biosciences.

In these areas, addressing the most compelling future science questions will require high flux neutron sources and techniques that exploit broader bandwidth, and improved resolution in energy and momentum. This can be achieved by taking advantage of the unique combination of complementary continuous and pulsed neutron sources available at ORNL. Key to our approach is optimizing the instrument suite over the entire complex including the High Flux Isotope Reactor (HFIR), the first target station (FTS) at the Spallation Neutron Source (SNS), and the planned second target station (STS) at the SNS. Our vision is to assure that the SNS and HFIR continue as world leading neutron scattering user facilities and centers of scientific excellence. Over the next decade we will achieve this by:

- Continuous engagement with the scientific community that will define the compelling scientific questions driving the development of our neutron facilities
- Integration with computation, synthesis, materials science, and biology efforts at ORNL to foster a multidisciplinary approach to neutron science
- Continued improvement in the neutron production from SNS and HFIR
- Optimizing existing instrumentation with targeted development of enabling technologies that will expand our current capabilities
- Providing innovative new capabilities and technologies (SING-III project)
- Building and operating a well-equipped second target station at SNS (STS)

Through community engagement, key elements of our strategic science plan are already underway. Instrument capabilities at SNS and HFIR are expanding, broadening the opportunities for science over increasing length, energy, and time scales. A growing suite of sample environments is allowing neutron research to be performed under more extreme conditions. Projects are underway to better integrate neutron sciences with high-performance computing for data analysis. STS received CD-0 approval and significant progress has been made toward the power upgrade project necessary to support the STS. Construction of the STS effectively leverages DOE's substantial investments in neutron science, and will deliver new scientific capabilities complementary to those of HFIR and the FTS.

This plan represents an update to the "Plan for Delivering High-Impact Science Using Neutrons, 2011." It is a living document and will be routinely amended as our strategy is implemented, workshop proceedings are completed and technological or scientific discovers are made.

DIRECTOR'S MESSAGE

Kelly Beierschmitt
Associate Laboratory Director for Neutron Sciences

On behalf of the staff of the Neutron Sciences Directorate at Oak Ridge National Laboratory (ORNL) and the science community that utilizes neutrons, I am delighted to present the 2014 update of the Strategic Plan for the Spallation Neutron Source (SNS) and the High Flux Isotope Reactor (HFIR). SNS and HFIR are unique scientific resources funded by the Department of Energy (DOE) Office of Basic Energy Sciences (BES) to accelerate discovery and learning in science and technology. These scientific user facilities exploit the neutron's fundamental physical properties to probe materials, and, thus, provide distinctive information about matter and energy. They provide information that is complementary to other probes used at BES user facilities, such as electrons and photons. In 2012, SNS and HFIR served more than 1,200 unique users who performed 800 experiments many in support of core BES missions.

SNS and HFIR support research to better understand, predict, and, ultimately control, matter and energy and are co-located with the Center for Nanophase Materials Sciences (CNMS) and the Oak Ridge Leadership Computing Facility (OLCF) at ORNL, a campus full of materials scientists, technicians, and engineers eager to collaborate with the broad user community. This research impacts many traditional and new innovative energy technologies, including new materials for lower heat loss, better electrical conduction, improved energy and fuel storage, energy efficient devices and machines, and new sources of energy such as solar conversion and biofuels. The energy challenge remains immense. Existing energy approaches and technologies will not be enough to secure our energy future or preserve our environment. This is precisely why such an environment for discovery has been created by the DOE. Meeting the challenge will require new technologies for producing, storing, and using energy, with performance levels that far exceed what is now possible, and, with concern to our planet, making all manufacturing and processing technologies environmentally friendly. Neutron scattering will continue to play a vital role in meeting these challenges.

The research we enable has a transformational impact on science. Consider the rapid advances in the study of multiferroics made possible by neutron scattering. Our ability to store and manage data on smaller scales has made possible the smart phone and other electronic devices that have changed our society. Yet, we have much to learn. Gaining a profound understanding of multiferroics could further advance the technologies associated with electronic devices in ways that we can only begin to image today.

I am humbled by the generation that has come before us – to think that the technologies we take for granted today were developed without the benefit of the neutron, photon, and electron sources available today. Slide rules were the norm, and supercomputers were only a dream. Moore's law suggests that in the last 40 years the number of transistors incorporated in the integrated circuit has doubled every two years. This has in part been made possible through the understanding we gain in materials using neutron scattering. In fact, many scholars have predicted the end of this exponential growth in computing power around 2020 due to limits in photolithography and current material knowledge. However, our scientists are imagining new ways for us to remove current physical limitations to perform operations on data through the direct use of quantum-mechanical phenomena such as superposition and quantum entanglement.

We seek to enable research that improves the human condition. I am fascinated, for instance, by what we do not understand of one of the most common and extensively studied substances on earth–water. It is vital for all known forms of life, but its unique behavior has yet to be explained in terms of the properties of individual molecules. Water derives many of its signature features from a combination of properties at the molecular level such as high polarizability; directional hydrogen bonding sites; and van der Waals forces. A profound understanding of the physics of water will greatly enhance our understanding of the mechanics of life.

The main objective of this plan is to continue the maturation of existing capabilities and establish a road map for introducing transformative capabilities that enable the science of the present and the science we can envision for the future. Continuous development of enabling technologies and their implementations at SNS and HFIR are important components to ensure the high performance of the facilities and are essential to continue meeting the ever changing needs of the scientific community. Through ongoing discussions with the community we have identified several key strategic science areas that will rely heavily on the unique characteristics of the neutron as a probe. We know today that there are capability gaps that prevent our community from advancing in certain areas of science. We aim to close these gaps through focused upgrades and innovative technological developments. Our priorities will be aligned to address the scientific needs of those that we support.

We work closely with our user community to understand the capability gaps that we must fill in today's scientific research. We must also look to the future to see what the important science drivers will be a decade from now and beyond. Science has made rapid progress over the past years in characterizing and understanding the detailed microscopic structure of matter. However, science is moving beyond a basic description of the arrangements and interactions of atoms and molecules that make up matter. As we move away from the atomic scale, complex architectures and interfaces at the nanoscale and mesoscale will emerge that have important new behaviors and functionalities that are difficult to explain using traditional quantum and classical physics. Understanding and controlling complexity will require exploring and characterizing nature across multiple length and timescales to discover new physical rules that connect the behavior of matter. This will require completely new types of neutron instrumentation designed to investigate emergent complexity, surfaces, and interfaces across vast ranges of length, time, and energy. Therefore, this plan also commits to a series of workshops to imagine and discuss the needs of the future.

I recognize that our goals and plan are ambitious. However, they reflect the ambitions of the scientific community we enable, and their success will be necessary for our collective future. I am grateful to this community and inspired by their ideas.

This plan envisions a decade or more of intense work. It is my hope that as we realize the vision contained within it, through the quality of our efforts we can not only exceed the expectations of our scientists, but just maybe change the way that they and we think about the science itself.

INTRODUCTION

This report outlines an ambitious strategic science plan that will be executed over the next decade to place the United States at the forefront of neutron science for at least the next two decades. ORNL operates two distinctive, powerful neutron facilities for DOE. Together these facilities are potent tools for understanding materials and energy and their conversion, synthesis, and control. The strategy calls for new and unique capabilities to be introduced at ORNL's SNS and HFIR advanced research user facilities. An immediate objective of the plan is to close neutron scattering capability gaps that are impeding progress in our science priority areas. The longer term vision is to continue to build the neutron scattering facilities of tomorrow that will be essential for overcoming the scientific challenges that the United States will face a decade from now and beyond. These neutron scattering activities will lead to the discovery of new phenomena and the formulation of the physical laws that govern complexity. The impact of our plan will be the development of transformative technologies for producing, storing and using energy.

ORNL Neutron Scattering User Facilities

The scientific breakthroughs that transform our future are accelerated by the availability of advanced research user facilities [1]. The DOE BES maintains 16 user facilities, including synchrotron radiation light sources, high-flux neutron sources, electron beam microcharacterization centers, and nanoscale science research centers [2]. BES installations enable progress in energy-related scientific and technological research and are used by more than 14,000 researchers annually, from disciplines including chemistry, physics, geology, materials science, environmental science, biology, and a wide range of engineering fields. The facilities make possible experimental studies that cannot be conducted in ordinary laboratories, enabling leading-edge research that benefits from a merging of ideas and techniques from different disciplines. At ORNL, BES has provided the nation with four user facilities: CNMS; the electron beam Shared Research Equipment Research (SHaRE) Center (to merge with the CNMS by 2015), and the two forefront neutron scattering user facilities, SNS and HFIR [2].

SNS and HFIR are vital and unique tools for scientific discovery and innovation because of the neutron's fundamental physical properties. Neutrons have wavelengths comparable to atomic and molecular length scales and are electrically neutral, strongly penetrating, and energetically well matched to elementary excitations in matter. Neutrons are especially sensitive to light elements in the presence of heavy ones, with the difference between hydrogen and deuterium being of particular importance. Neutrons have a magnetic moment and are hence sensitive probes of magnetic ordering and excitations. Finally, neutron scattering is very directly connected to a host of phenomena and its quantitative measurement enables a very direct comparison with theoretical and computational modeling, offering deep insights into the behavior of complex matter.

The new knowledge and access to phenomena provided by neutrons complements that from the other probes such as electrons and photons available at other BES research user facilities. Neutrons see atoms and ions, they see differences in isotopic composition, they follow motions, and they reveal magnetic and electronic properties that are all but invisible to electrons and photons. Neutrons can be used to probe the enormous range of length and timescales involved in complex materials and systems that are emerging as major scientific challenges in the twenty-first century. Further, neutrons can penetrate deep into bulk materials with enhanced contrast to detect physical phenomena at interfaces and surfaces that underpin new devices and technologies. Neutrons are complementary to photons for studying the structure of hydrogenous systems and can probe the detailed properties of water and the interactions of water with other molecules, atoms, and ions that are crucial to materials and energy and to our understanding of cellular processes that form the basis for the physics of life. Finally, neutrons will always be complementary to photons for studying dynamic processes.

Neutron beams suitable for scattering experiments cannot be generated in small-scale academic or industrial laboratories; thus large-scale user facilities are the only means of providing neutron beams to the scientific community to access their unique possibilities. Neutrons play an essential role in addressing BES research missions and grand science challenges; this has been stated in the reports from every BES-sponsored "Basic Research Needs" research community workshop over the past decade [3].

Neutrons are generated continuously in steady-state via fission at HFIR. At the SNS a pulsed accelerator is used to generate protons that strike a mercury target to spall pulses of neutrons, enabling highly efficient use of the neutrons in time-of-flight experiments. SNS and HFIR therefore have complementary characteristics: the SNS is pulsed with a high peak flux and HFIR is continuous with a high time-averaged flux. Neutrons produced at the SNS and HFIR are guided to a variety of different specialized instruments. Crystallography, small-angle scattering, diffraction, reflectometry and imaging beam lines are ideal for studying structure and magnetic organization from the atomic to micrometer length scales. Neutron spectroscopic beam lines characterize self- and collective motions and excitations from sub-picosecond to microsecond timescales. In 2012, the SNS and HFIR operated 24 beam lines that served more than 1200 unique users who performed 800 different experiments. As world-class user facilities, they serve a broad range of users proposing peer-reviewed forefront research in physical, chemical, materials and life sciences. BES-supported individual investigators, BES Energy Frontier Research Centers (EFRC) scientists, and DOE-supported research and development programs utilize the facilities to support DOE missions. Additional beam lines are coming on-line as the SNS Instruments Next Generation (SING) programs for instrument construction are completed. The current set of instruments is listed in Table 1.

ORNL neutron scattering instruments currently available			
SNS		HFIR	
Beam line	Instrument	Beam line	Instrument
1B	NOMAD: Nanoscale-Ordered Materials Diffractometer	CG-1	Development Beam Line
2	BASIS: Backscattering Spectrometer	CG-1D	IMAGING: Neutron Imaging Prototype Facility
3	SNAP: Spallation Neutrons and Pressure Diffractometer	CG-2	GP-SANS: General-Purpose Small-Angle Neutron Scattering Diffractometer
4A	MR: Magnetism Reflectometer	CG-3	Bio-SANS: Biological Small-Angle Neutron Scattering Instrument
4B	LR: Liquids Reflectometer	CG-4C	CTAX: Cold Neutron Triple-Axis Spectrometer
5	CNCS: Cold Neutron Chopper Spectrometer	CG-4D	Imagine: Quasi-Laue diffractometer at HFIR
6	EQ-SANS: Extended Q-Range Small-Angle Neutron Scattering Diffractometer	HB-1	PTAX: Polarized Triple-Axis Spectrometer
7	VULCAN: Engineering Materials Diffractometer	HB-1A	FIE-TAX: Fixed-Incident-Energy Triple-Axis Spectrometer
11A	POWGEN: Powder Diffractometer	HB-2A	Powder: Neutron Powder Diffractometer
12	TOPAZ: Single-Crystal Diffractometer	HB-2B	NRSF2: Neutron Residual Stress Mapping Facility
13	FNPB: Fundamental Neutron Physics Beam Line	HB-2C	WAND: US/Japan Wide-Angle Neutron Diffractometer
14B	HYSPEC: HYSPEC---Hybrid Spectrometer	HB-3	TAX: Triple-Axis Spectrometer
15	NSE: Neutron Spin Echo Spectrometer	HB-3A	FC: Four-Circle Diffractometer
16B	VISION: Vibrational Spectrometer		
17	SEQUOIA: Fine-Resolution Fermi Chopper Spectrometer		
18	ARCS: Wide Angular-Range Chopper Spectrometer		

Table 1: A list of instruments in the HFIR and SNS user programs as of October 2013. There is an alignment station at CG-1B at HFIR which is not included in the table.

Beam line scientists are the primary link between facility operations and scientific impact, and this plan is based on scientific staffing that meets the needs of expanding facility capabilities. Beam lines also depend on state-of-the art enabling technologies including hardware components such as choppers, detectors, neutron optics and sample environments, and software components and computational methods for instrument control, data acquisition, analysis, and visualization. The co-location of the SNS and HFIR with the powerful high performance computers of the DOE OLCF provides an opportunity to fully integrate neutron scattering with high performance computing, and co-location with the CNMS user facility allows for an integrated BES user program of nanophase materials synthesis, laboratory characterization, theory, modeling and simulation, and neutron scattering. There has been a rapid increase in the number of users, demand for beam time, and scientific productivity at the SNS and HFIR over the past five years. Demand for experimental access at the SNS and HFIR already exceeded capacity by a factor of 2-3 in 2012. By 2018 the completed suite of beam lines is expected to be over-saturated with high-quality experiments.

The SNS and HFIR are part of a national infrastructure of neutron user facilities that includes the BES Lujan Neutron Scattering Center (the Lujan Center) at the spallation source operated by Los Alamos National Laboratory (LANL) and the National Institute of Standards (NIST) Center for Neutron Research (NCNR) at the reactor source operated by the Department of Commerce (DOC). Over 20 neutron research facilities operate worldwide. The landscape of advanced neutron research facilities worldwide is changing at the moment in response to the rapidly evolving nature of twenty-first century science and technology that will focus on the nature of complex materials. Over the next decade new next-generation spallation neutron sources will be completed, including the European Spallation Source (ESS) and the Japan Proton Accelerator Research

Complex (J-PARC). The ESS and J-PARC have been designed to have strengths for understanding the nature of complex materials. A comparison of key parameters of ORNL capabilities and other leading international neutron research facilities is discussed below.

The SNS and HFIR will benefit from closer partnership with other BES facilities in joint user programs. Forefront science depends on increasing integration of different types of information from complementary synthesis, characterization, theory, and computational research tools. Users regularly complement data collected on SNS and HFIR beam lines with X-ray, microscopy, transport, susceptibility, or NMR data and with data from complementary beam lines at other neutron sources such as LANSCE and NCNR. There are also advances in enabling technologies that can benefit several experimental methods. The SNS and HFIR will align and partner with other research facilities whenever possible to develop the best solutions to science and technology development.

Comparison with Leading International Neutron Facilities

BES has positioned ORNL as the only place in the world with a co-located operating high-flux research reactor and spallation neutron source. Typically, experiments that require high integrated fluxes of neutrons at long wavelengths (such as small angle neutron scattering) or that concentrate on a relatively small range of energy-momentum phase space (such as triple axis spectroscopy) depend primarily on time-averaged source brightness integrated over the wavelength band of interest—a strength of continuous neutron sources such as HFIR. The cold source at HFIR produces a high flux of long wavelength neutrons comparable to the world's best reactor cold sources (e.g. the Institute Laue Langevin) shown in Figure 1a and provides the highest time-averaged flux of cold neutrons of the ORNL sources. HFIR will maintain its leadership position in this domain even after ESS and J-PARC have been built and have achieved their design performance.

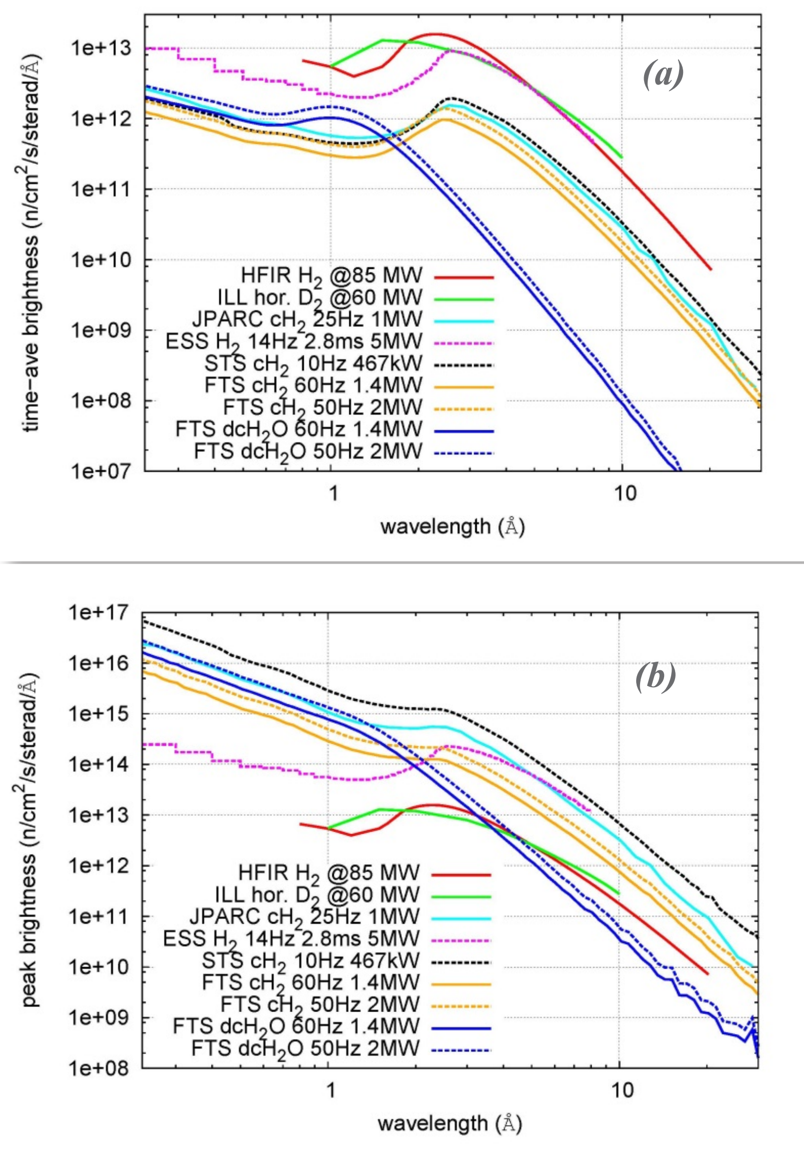

Figure 1. Moderator and cold source performance from leading and proposed reactor and pulsed spallation neutron sources. Solid curves represent the full baseline performance of existing sources while dotted-dashed curves represent future facility plans. The upper plot (a) shows the time averaged brightness of the moderators and cold sources while the lower plot (b) shows the peak brightness The performance of some neutron scattering instruments scales with the average flux as in (a), while others scale with the maximum number of neutrons that can be generated over a short period of time as in (b). The performances of remaining instruments scale somewhere between these two extremes.

At the other extreme, experiments that require good wavelength resolution and use either a broad incident wavelength band (such as powder or single crystal diffraction) or a broad scattered wavelength band (such as chopper spectrometers) depend primarily on the peak source brightness—a strength of spallation neutron sources such as the SNS FTS, Figure 1b. SNS FTS provides some of the highest peak brightness available worldwide. The accelerator power upgrade that will be part of SNS STS will increase FTS performance by roughly 40 percent compared with operation at the current design power (1.4 MW). However, J-PARC– which has not reached its design performance– is already beginning to outperform SNS FTS in peak brightness at most wavelengths. The planned ESS will outperform the SNS FTS in peak brightness at the long wavelengths of cold neutrons. Our strategic science plan includes a proposal to build a STS, envisioned to be a long wavelength, short pulse source with a 10 Hz pulse rate and 400–500 kW proton beam power. With these parameters the SNS STS would have the highest peak brightness of any existing or planned neutron source.

Optimizing many classes of experiments depends on linking source characteristics and instrument design to the scientific problems. For example, characterizing materials and interfaces simultaneously in a time-resolved manner over multiple length scales from the atomic through to the mesoscale and beyond is a key goal of research in complex systems. This type of experiment requires high peak brightness over a very broad dynamic range of length scales. The low pulse-repetition rate of the planned STS is designed to achieve this broad dynamic range. More detailed comparisons of existing and planned neutron sources are given in the Appendices.

Strategic Planning and Research Community Involvement

Continuous development and upgrade of SNS and HFIR are critical to performance of these facilities and therefore of the strategic planning of both BES and ORNL. [2] BES involvement of the research community in this strategic planning process includes a committee that advises on research areas and user facilities – the Basic Energy Science Advisory Committee (BESAC). BESAC has produced several reports that outline basic research needs for neutron scattering that are required to ensure a secure energy future [3]. In a recent BESAC report, it was recommended that "Leadership in the science of materials is needed to ensure economic competitiveness and enable innovation. For the United States to lead in materials research, it must have world-leading neutron science capabilities." [4] After a review of SNS and HFIR in August 2012, BES requested that ORNL continue to develop a strategic plan to transform SNS and HFIR into centers of scientific excellence and world-leading neutron scattering user facilities.

ORNL is actively engaging the research community to participate in updating and refining its strategic science plan. Over the past decade several BES– and ORNL–sponsored studies and workshop reports produced by the research community have recommended construction of a SNS STS in order to extend the capabilities beyond SNS FTS and HFIR, to maintain United States leadership in neutron scientific research and innovation. A recent BESAC report on the prioritization of existing and proposed BES user facilities urged "the strong support of a major upgrade to DOE's premier neutron facility, SNS. SNS STS, and the associated power upgrade of SNS are both crucial to increase significantly the facility's capability and capacity. The STS will be absolutely central to United States world leading science" [4]. ORNL is ready to proceed with the design and construction of the STS, having received CD-0 approval from DOE in 2009. Consultation with the research community is ongoing to optimize STS parameters based on emerging scientific challenges and the evolving international landscape of competing advanced neutron sources.

In March 2013, ORNL asked its Neutron Advisory Board (NAB) to provide recommendations for a broad planning process intended to map out future developments at both SNS and HFIR. The NAB recommendations included convening a panel of external experts on future science impacts for neutrons (which took place in June 2013) with the goal to identify areas of science in which neutrons can provide vital information that cannot be obtained by any other technique. Further, NAB recommended organizing a series of focused scientific and technical workshops to produce reports refining those areas of future science priority and to identify new opportunities for neutron scattering in those areas. Results from future workshops will provide the foundation for further development of the strategic science plan for SNS and HFIR.

Workshops will also be organized to explore forming partnerships on beam lines with potential partners from agencies other than DOE in a cooperative stewardship model as recommended by a 2013 Committee of Visitors of the Scientific User Facilities Division of BES. In addition to DOE, other agencies, including the DOC, the National Science Foundation (NSF), and the National Institutes of Health (NIH) will be invited to participate in these workshops. The goal of the workshop is to map out the present and future needs of the United States scientific community for neutron scattering with a view toward meeting those needs with expanded novel instrumentation. To facilitate the workshop process, SNS and HFIR staff will develop a documented suite of instrument specifications for new and upgraded beam lines at HFIR and the existing SNS FTS by spring 2014. The documented suite will also include possible beam lines for the planned STS. This continuing process of involvement is designed to ensure that the upgrade and development of SNS and HFIR include instrumentation addressing the needs of the research community.

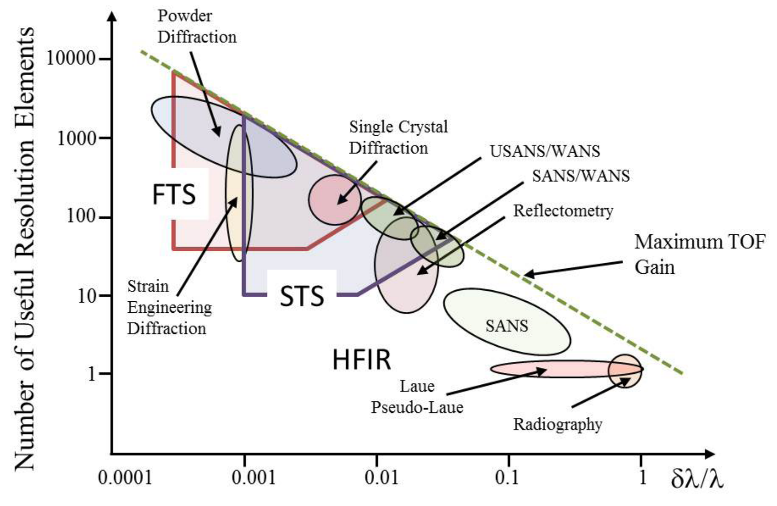

Figure 2. Optimal performance map of elastic scattering instruments across the ORNL neutron sources. The horizontal axis is the wavelength resolution of the indicated instrument types (shaded ovals) while the vertical axis is the number of these resolution elements that are required for any given measurement. The dashed green line establishes the maximum performance gain that can be achieved with TOF techniques used by all the neutron scattering instruments at the ORNL pulsed sources. Within their respective labeled boxes, we expect the performance of the SNS FTS and STS target stations to exceed that of HFIR. Outside the boxes, HFIR will obtain a desired data set more quickly. The boundaries between HFIR and the pulsed sources are established as the level at which gains in using TOF techniques are matched by the higher time-averaged flux of HFIR.

New Opportunities

The central principle of ORNL's strategic science plan for SNS and HFIR is the formulation of science priorities that in turn drive the development of new and upgraded beam lines, sources and enabling technologies. Capitalizing on this opportunity will provide unparalleled efficiency in the scientific discovery needed for BES missions, and will contribute to the international preeminence of the entire neutron facilities complex in the United States. For example, as Figure 2 illustrates, most diffraction instruments used to characterize relatively small structures are better positioned at SNS FTS, whereas small angle scattering instruments that are used to characterize large–scale structures at a particular length scale are better positioned at HFIR. Instruments that are well-matched for HFIR and SNS FTS will be upgraded to maximize their performance and extend their scientific reach.

There are capability gaps that are limiting our ability to address today's science priority areas and those of the future to characterize complex materials and interfaces across broad ranges of length, time, and energy. These gaps can only be closed by developing new types of beam lines, best positioned to take advantage of the broad bandwidth and high intensity of the STS. Relevant instruments include reflectometers, small and wide angle neutron scattering (SANS/WANS) instruments and ultrasmall angle neutron scattering (USANS) instruments. Diffraction instruments optimized to characterize large structures or magnetic systems and inelastic instruments that access low energies and long timescales would also be better positioned at STS. Backscattering spectrometers that probe local diffusional motions could cover different dynamic ranges and resolutions at STS, FTS, and HFIR. Building additional quasielastic scattering instruments at STS and HFIR would extend the reach of this technique to slow relaxations and longer length scales beyond what is currently possible at FTS. Instruments that survey broad areas of energy and momentum transfer depend primarily on peak brightness at the wavelength of interest. Therefore, cold neutron instruments of this type would perform almost an order of magnitude better at STS than at HFIR.

The strategic timeline for these developments is provided later in the document and envisages a continual optimization of beam lines across sources to maximize their performance and scientific impact over the next 10 years. This timeline consists of phased and interconnected developments, and has the built-in flexibility to be responsive to changes in national materials research and BES scientific priorities as they are continually refined through consultation with key stakeholders. This flexibility reflects the fact that our scientific understanding of the world evolves in leaps that are not easy to predict. Notwithstanding this uncertainty, we can anticipate and plan for significant advances in some key areas of science as described in the next section.

References

1. US DOE Office of Science Strategic Plan, February 2004, DOE/SC-0079.

2. US DOE Office of Science, Basic Energy Sciences 2011 Summary Report. DOI: http://energy.gov/sites/prod/files/2011_DOE_Strategic_Plan_.pdf.

3. BESAC and BES have engaged thousands of scientists from academia, national laboratories, and industry from around the world to study the current status, limiting factors, and specific fundamental scientific bottlenecks blocking the widespread implementation of alternate energy technologies. The reports from the foundational Basic Research Needs to Assure a Secure Energy Future workshop, the following ten "Basic Research Needs" workshops, the panel on Grand Challenge science, and the summary report *New Science for a Secure and Sustainable Energy Future,* (BESAC, 2008: http://science.energy.gov/-/media/bes/pdf/reports/files/nssset_rpt.pdf) detail the key basic research agendas needed to create sustainable, low carbon energy technologies of the future. These reports have become standard references in the scientific community and have helped shape the strategic directions of the BES-funded programs. DOI: http://science.energy.gov/bes/news-and-resources/reports/.

4. *The Basic Energy Sciences Facilities Prioritization* report is a result of a BESAC subcommittee meeting February 26–27, 2013; DOI: http://science.energy.gov/~/media/bes/besac/pdf/Reports/BESAC_Facilities_Prioritization_Report_2013.pdf.

SCIENCE PRIORITIES

Neutrons are a precious and irreplaceable scientific resource. They follow the quantum mechanical spin of the electron in solids, can penetrate sample chambers to look at materials under extreme conditions and provide unique information about the building blocks of life. Through a process of ongoing consultation with ORNL staff, users, expert advisory committees and workshops involving the broader research community, science priority areas have been identified with research challenges and opportunities that can be best addressed by the unique and vital information provided by neutron scattering. These promising directions for future neutron scattering, discussed in this section, are driving the technology decisions of ORNL's strategic science plan for SNS and HFIR.

Introduction

Our primary motivation is to deliver the scientific tools that provide solutions to United States energy challenges that make up the core missions of the DOE Office of Science. We have identified key science priorities – quantum materials, materials synthesis and performance, soft molecular matter, and biosciences – that represent areas where strong overlap exists between the capabilities of neutron sciences and the vast scope of these energy-related challenges. In addition, the reach of neutron sciences in these priority areas naturally extends beyond energy challenges and can address a diverse array of compelling scientific problems limited only by the imaginations of scientists. Part of our strategic science plan will drive the development and upgrade of SNS and HFIR capabilities to close capability gaps in our science priority areas, providing new opportunities for making scientific breakthroughs.

The technologies and materials of tomorrow will depend on understanding and manipulating how atoms and molecules combine to create complex architectures at the nanoscale and mesoscale that have new behaviors and functionalities. The general need to understand and control complexity will impact all of our science priority areas and requires exploring and characterizing nature to discover new physical laws that connect the behavior of matter across lengthscales and timescales. With new sources, instrumentation and simulation/modeling, it becomes possible to step into this new level of complexity and explore the most elusive realms of biosystems in action and the quantum properties of matter on mesoscopic scales. The possibilities for important new materials are endless and will capitalize on advances in chemistry, condensed matter physics, and biology. One can anticipate that these advances will be based on manifestations of quantum effects, mesoscopic microstructures, with inspiration from biology or possibly with materials including biological components. Our vision is to optimize and combine the capabilities of HFIR, FTS, and STS into the world's most powerful array of neutron capabilities and focus these on the forefront challenges of the coming decades.

Quantum Materials

Some of the most exciting novel materials that could lead to transformational technologies are those where useful macroscopic properties originate from explicitly quantum effects. Such materials have the potential to result in new, more energy efficient technologies for next generation electronic devices. Many of the most technologically interesting materials exhibit couplings of multiple degrees of freedom. Prime examples include multiferroic or spintronics systems based on metals, oxides, or organics which have a range of potential applications including magnetic field sensors, low power memory modules, high density storage devices, and quantum computing. These materials are important components of the infrastructure for energy technologies at all levels. A central goal for fulfilling DOE's energy mission is to characterize and understand such materials.

Research on quantum materials addresses several of the scientific "grand challenges" that have been identified by DOE [1] and the National Academy of Sciences (NAS) [2] committees with particular relevance to the following questions:

- How do we control material processes at the level of electrons?
- How do remarkable properties of matter emerge from complex correlations of atomic or electronic constituents and how can we control these properties?
- How do complex phenomena emerge from simple ingredients?

Historically neutron scattering has played a key role in defining many of the fundamental concepts that have provided an understanding of conventional materials, ranging from establishing the reality of quantized collective excitations such as phonons and magnons to the idea of broken symmetry in phase transitions. Today, neutron scattering is a central technique for addressing modern grand challenges in condensed matter physics [1]. Neutron scattering will remain a unique and indispensable tool for studying new aspects of quantum materials for the foreseeable future, but new concepts and major improvements in neutron sources and instrumentation are called for to address the frontier problems of tomorrow.

Currently, SNS and HFIR have a diverse suite of instruments used in the study of quantum materials on multiple length scales and the underlying microscopic interactions on multiple energy scales. Neutron scattering on these instruments has led to better understanding of the role of magnetism in high temperature superconductors, the microscopic interactions responsible for multiferroicity, the emergence of exotic, quantum states from specific structural motifs, and the relationship between magnetism and heat transport. Many of the phenomena at the forefront of quantum materials research involve magnetism and its coupling with the underlying lattice. The sensitivity of neutron scattering to both magnetic and lattice degrees of freedom make it an indispensable tool in such investigations. Neutrons are also valuable for determining the atomic structure of novel materials and for mapping atomic vibrations, which play an essential role in a diverse range of functional materials such as thermoelectrics and superconductors [3].

Scientific challenges

Understanding how unexpected properties of matter emerge from complex correlations of the electronic constituents remains a BES grand challenge. Control of these properties can lead to new functional devices. One prototypical example is giant magnetoresistive devices where the manipulation of spin can be used to control charge: such devices and those related technologies (e.g., tunneling using magnetoresistance) are now ubiquitous in the information storage industry. Magnetism itself is a manifestation of strong correlations, and many of the materials exhibiting emergent exotic behavior also tend to exhibit static and/or dynamic magnetism. The sensitivity of neutron scattering to magnetic moments makes it a unique tool in the study of such materials, and it has played a significant role in the comprehension of many emergent phenomena. However, problems of interest are increasingly complex, often involving coupled spin, orbital, and lattice degrees of freedom and magnetic electrons that vary from local to itinerant. The detailed understanding of such complex materials poses significant challenges. One specific example is the area of multiferroics, where ferroelectricity is tightly coupled to magnetism, potentially allowing the control of electric properties with magnetic fields or vice versa. While neutrons have yielded detailed understanding of the microscopic magnetic properties, the coupling of the lattice to the magnetic subsystems has not been quantitatively explored due to the complexity of the coupled system and its resulting excitations. To do this

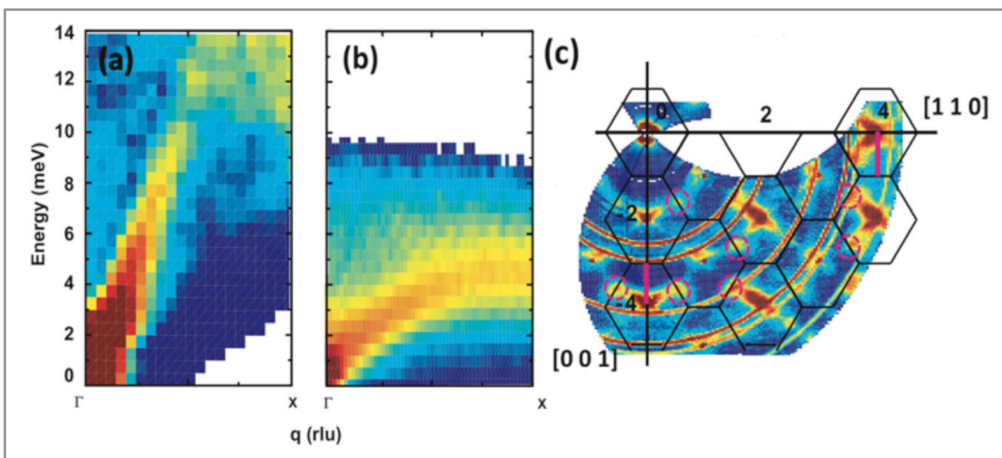

Figure 3. Understanding thermal conductivity is important in various energy related technologies from building insulation to heat exchangers to nuclear reactor fuels. Modern inelastic neutron scattering instruments provide a unique, microscopic view of thermal conductivity via measurements of phonon dispersions and lifetimes over a full Brillouin zone. For thermoelectric materials, low thermal conductivity is important and inelastic neutron scattering measurements were used to understand the nature of the glass-like thermal conductivity in $AgSbTe_2$. These measurements, combined with diffuse scattering and electron microscopy revealed that naturally occurring nanostructures are responsible for the low thermal conductivity of this material. This mechanism could provide a pathway to the discovery of new materials with enhanced thermoelectric properties. J. Ma et al., "Glass-like phonon scattering from spontaneous nanostructure in $AgSbTe_2$," Nature Nanotechnology 8, 445 (2013). (ARCS, CNCS, and POWGEN of SNS, and HB-3, HB-1A, and CTAX of HFIR.)

effectively requires spectroscopic methods that cover wide areas of momentum space with excellent resolution in energy and momentum.

Elucidating the mechanisms underlying high-temperature superconductivity [3] in copper- and iron-based superconductors remains a significant challenge at the forefront of materials research. Superconductivity has the potential to dramatically change the capacity, efficiency, and reliability of the power grid, and a goal of basic research is a materials-by-design approach to developing new, improved superconductors with optimized transition temperatures and current-carrying capabilities. However, such optimization requires an understanding of the pairing mechanism in these materials, and while significant experimental and theoretical progress has been made, such understanding remains elusive. Neutrons are ideally suited to study magnetism, which is believed to play an important role in the superconducting pairing mechanism in these materials. At the same time, neutrons are sensitive to the lattice and orbital degrees of freedom, which may also be important to this emergent state. In addition to understanding the pairing mechanism, states in close proximity to high-Tc superconductivity in cuprates display unusual "non-Fermi-liquid" behavior. Understanding the role of the pseudogap that defines this state remains a significant challenge that may, ultimately, shed light on the nature of the pairing.

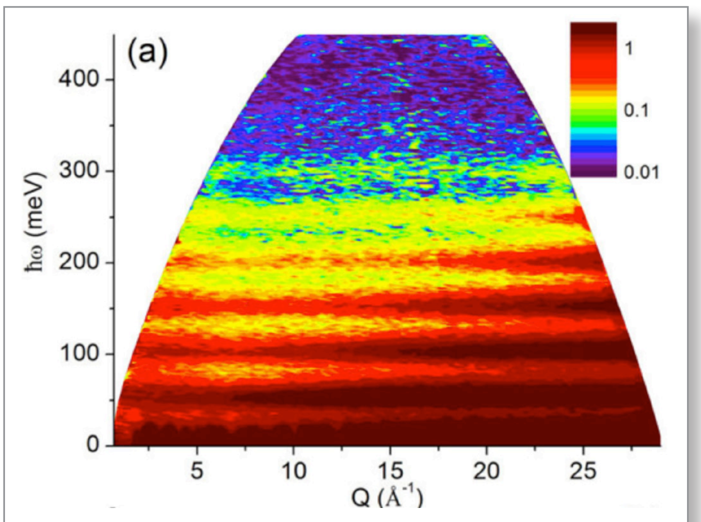

Figure 4. Inelastic neutron scattering measurements of uranium nitride (UN) at SNS allowed extension of previous studies to much higher energies revealing a set of evenly spaced energy levels extending to at least 500 meV. The measured data are quantitatively consistent that of a single atom, isotropic harmonic oscillator resulting from nitrogen atoms oscillating in the octahedral cage of heavy uranium atoms. This observation demonstrates that the best experimental realization to date of a single atom behaving as the exactly solvable, three-dimensional quantum harmonic oscillator. UN has been considered as potential fuel in generation IV nuclear reactors and these previously unknown high energy modes may be important for understanding the total neutron cross-section in such reactor designs. A. A. Aczel et al., "Quantum oscillations of nitrogen atoms in uranium nitride," Nature Communications 3, 1124 (2012). (Data shown here from SNS ARCS at SNS, the experiment also used SNS SEQUOIA).

Another BES grand challenge is the quantum control of electrons in atoms, molecules, and materials. One of the simplest routes to such control is via manipulation of electron spin. For this reason correlated materials where magnetism is coupled to charge, lattice, or orbital degrees of freedom are of particular interest. As described previously, neutrons play an important role in understanding the fundamental properties of such materials. The understanding of magnetic excitations in materials has moved beyond the original simple models of "spin waves," and neutrons can now be effectively used to probe more exotic phenomena including quantum states in molecular magnets and fractional excitations in low dimensional quantum spin systems. These materials have

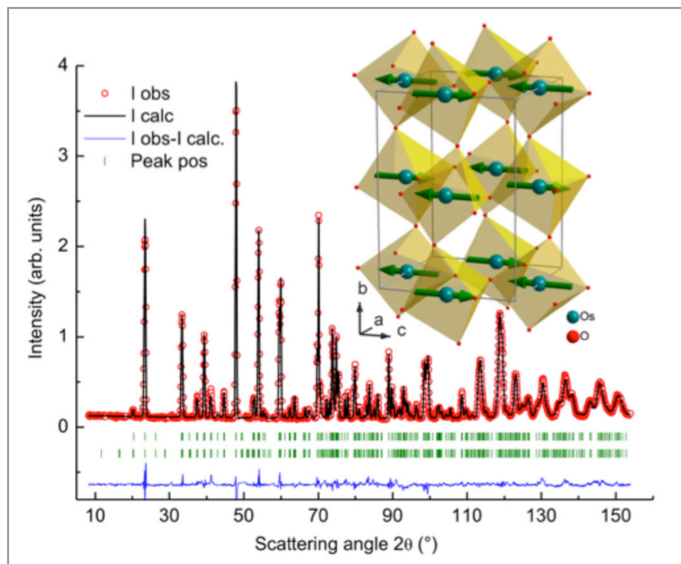

Figure 5. A metal-insulator transition driven by long-range magnetic order was proposed by Slater in 1951, but an experimental verification of this mechanism has remained elusive. Combined X-ray and neutron diffraction measurements of the crystal and magnetic structure of $NaOsO_3$ provide the first definitive experimental demonstration of the Slater mechanism for a metal-insulator transition in a real material S. Calder et al., "Magnetically driven metal insulator transition in $NaOsO_3$," Physical Review Letters 108, 257209 (2012). (Data shown here from HB-2A at HFIR; the experiment also used HB-1).

potential for quantum computing applications; meanwhile an efficient exploration of excitations in these materials requires neutron instruments covering a large range of energy scales from microelectron volts (μeV) to electron volts (eV). Exploring the properties of quantum materials in nonequilibrium conditions, as may be appropriate for real device applications, is an important scientific frontier. Such studies are challenging experimentally, requiring the development of novel pump-probe sample environments and the use of advanced theoretical approaches to understand non-equilibrium quantum systems.

DOE's Critical Materials Strategy [4] calls for the development of next generation permanent magnets that are less reliant on the specific rare earth metals used in today's technology. This demands a detailed understanding of magnetism at multiple length scales, for which neutron scattering will play an essential role. As described previously, neutrons facilitate understanding of both static and dynamic microscopic interactions, but the properties of magnetic materials are also strongly affected by their mesoscale magnetic domain structures. The statistically averaged structure of such domains can be determined using polarized SANS and reflectometry techniques. Instruments specialized for these measurements will impact numerous forefront problems in hard matter physics. For example, thin film oxides manifest a wide range of unexpected phenomena due to reduced dimensionality, strain, defect chemistry, and exchange bias. These materials may form the basis of future "oxide electronic" technologies with the potential for major gains in energy conservation and qualitatively new devices using the electron's spin as well as charge. Polarized reflectometry provides a unique ability to determine magnetic structure through the film and in particular at buried interfaces. An important instance where mesoscale phenomena determine function is the vortex state of high temperature superconductors, which limits the current carrying capability of superconducting wire. SANS provides an excellent tool for examining these vortex lattices and the distribution of vortices in the presence of pinning. To optimize function, magnetic domain structures and vortex lattices should be studied in operando and with time-resolved techniques to understand domain wall or vortex motion and allow tuning of properties for applications.

An optimized instrument suite across HFIR, FTS and STS would provide access to an unprecedented range of length scales and timescales enabling the study of new materials. Increasingly, interesting phenomena are being observed

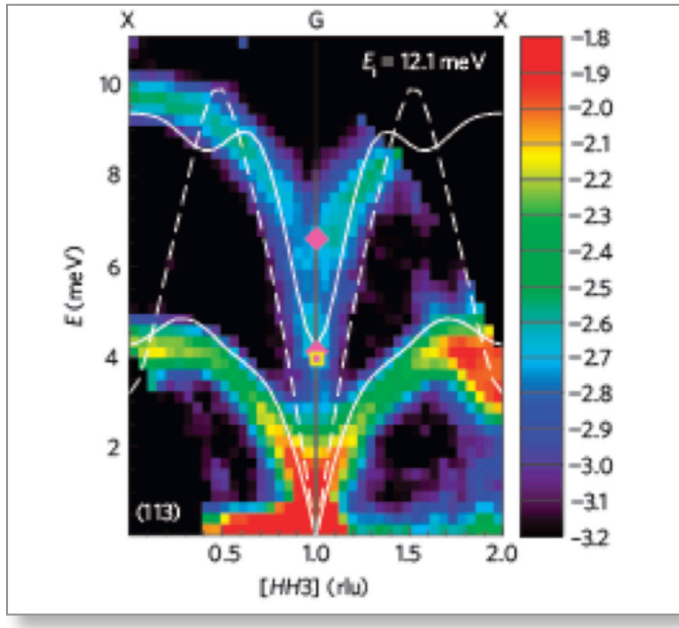

Figure 6. Inelastic neutron scattering studies of phonons are crucial for understanding the microscopic origins of thermal conductivity in thermoelectric materials, which offer great potential for more energy efficient devices. Measurements in PbTe revealed a giant anharmonic coupling between a "ferroelectric" optic mode and longitudinal acoustic mode. This explains the low thermal conductivity of PbTe shows why many good thermoelectric materials occur near ferroelectric lattice instabilities. O. Delaire et al, "Giant Anharmonic Phonon Scattering in PbTe,"Nature Materials 10, 614 (2011). (Data shown here from SNS CNCS; the experiment also used HB3 at HFIR).

at longer length scales, with the observation of novel topological states of matter such as skyrmion lattices being a recent example. Typically these larger objects are characterized by lower energy excitations so that investigating excitations of mesostructures requires cold neutrons. In general, despite progress toward materials-by-design, most new materials are still discovered in an ad hoc manner. An optimized suite of instruments covering a large range of length scales and timescales, enabling technologies like sample environment, and a strong link to theory and computation would increase the impact of neutron scattering, keeping researchers at the forefront of materials research.

Capability Gaps and Opportunities

As is well known, the relative weakness of neutron scattering cross sections means that many measurements are flux limited. New neutron sources and instrumentation using optimal moderators and optics to enhance useful flux on samples directly benefit wide areas of science and open up new problems to useful investigation via neutron scattering. Many of the near-term upgrade plans and development efforts at ORNL are aimed at improving this flux. Flux improvements will benefit almost all areas of quantum-materials-related research.

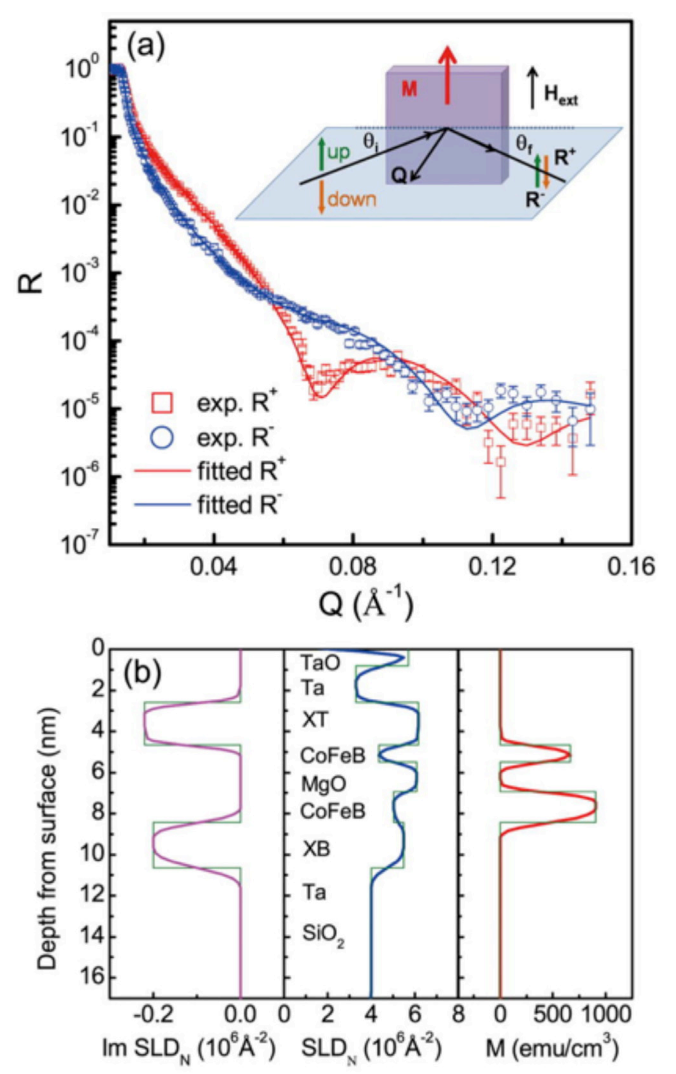

Figure 7. Low-D magnetoelectronics. Reduced-dimensionality structures offer direct control of both magnetic and electronic degrees of freedom, and an exciting path to the development of novel devices. Polarized reflectometry opens new opportunities for studying epitaxial thin films, multilayer structures, and interfaces. (a) Polarized neutron reflectivity of a buried CoFeB layer. (b) Depth dependence of scattering length density and magnetization. The results reveal an asymmetry in the magnetization of the CoFeB layer above and below the magnetically dead MgO later. T. Zhu et al., "The study of perpendicular magnetic anisotropy in CoFeB sandwiched by MgO and tantalum layers using polarized neutron reflectometry," Applied Physics Letters 100, 202406 (2012). (SNS Magnetismsim Reflectometer)

Novel, emergent phenomena are increasingly characterized by mesoscopic-scale structures [5]. Moreover, the actual behavior of materials as well as devices using them is often dominated by defect and domain structures with length scales exceeding the atomic but not macroscopic: the regime of mesoscale phenomena. Current instrumentation has a limited ability to simultaneously take data over a large range of length scales; improving this capability will open up new areas of structural science. For quantum materials this will yield particular advantages for examining mesoscale magnetic structures, such as skyrmion lattices, orbital currents in unconventional superconductors, vortex lattices, and nanoscale electronic phase separation including striped phases in copper-oxide superconductors. The pulsed source combined with event mode data handling also opens up the realm of time-resolved pump-probe experiments that can be applied to nonequilibrium situations. In the long term, optimal instruments will have sufficient intensity to rapidly resolve in-plane magnetic superstructures in thin films or devices with much better dynamic range opening up the possibility of in situ measurements of spintronic devices under operating conditions. This will enable new science that is complementary to that afforded by x-ray scattering or imaging techniques.

Many of the most compelling problems in condensed matter physics require investigations of collective excitations using low energy measurements with excellent resolution. In many situations the important physics is strongly coupled to a specific wave vector and is ideally investigated using a spectrometer based at a continuous cold source that can be specifically optimized for the measurement. In other instances many length scales and energy scales are important, placing a high premium on broad-bandwidth, high-resolution cold neutron spectrometers. The emergent mesoscale structures discussed previously are typically characterized by low-energy fluctuations, requiring a high intensity of cold neutrons. A detailed understanding of emergent physics at quantum critical points remains one of the most pressing problems in condensed matter physics. Investigating the quantum critical state demands ultra-low-temperature capabilities combined with high pressure and high magnetic fields. Characterizing the critical behavior requires the investigation of fluctuations in energy ranges 1μeV to 10 meV and a full range of momentum transfers, with emphasis on low Q < 3 inverse angstroms. The problem of frustrated magnetism, where conventional magnetic order is incompatible with conflicting interactions at the atomic scale, is another excellent example demanding these capabilities. Synergistic progress in theory and experiment in the past five years has resulted in the discovery of such phenomena as magnetic monopole excitations.

Systems where ground states and excitations are determined by topological properties are increasingly important and often exhibit new phenomena such as fractional excitations that may span a wide energy range, calling for optimized inelastic instruments at FTS, STS, and HFIR. Many topological states under investigation now arise from strong spin-orbit coupling, and an important frontier area that is now opening up involves systems with 4d, 5d, and possibly 6d electrons where strong spin-orbit coupling combined with covalency leads to new physics. The extended nature of the magnetic electrons in such systems requires measurements at small wave-vectors to avoid form-factor suppression of the magnetic signal.

The low-energy and low-temperature measurements required to investigate much of the new physics discussed above is challenging today for neutrons and will be very difficult to investigate effectively with photons. However, it is well matched to the greatly improved cold neutron TOF spectrometers planned for the future. The next-generation low-energy chopper instruments planned for STS will combine its high flux at cold and thermal neutron energies with greatly improved signal to noise and advanced multiplexing to acquire information on both structure and dynamics through a hierarchy of length scales and timescales. For problems where the important science is dominated by a restricted portion of energy – momentum phase space, the spectrometers at HFIR can be optimized, providing key measurements complementary to those obtained using TOF methods.

Many of the most compelling scientific problems in quantum materials can best be addressed by probing materials under extreme conditions of temperature, pressure, or field [6]. Neutron scattering is well-matched to these measurements, but in some instances the necessary sample environment has not been developed or is not readily available. Combining the source-related advantages mentioned above with new sample environments such as extreme low temperatures, high pressures, and high magnetic fields is precisely what is required to expose intriguing new phenomena in materials. Our strategy calls for developing the necessary sample environment capabilities as well as spectrometers.

In particular, the combination of neutron scattering and high magnetic fields is expected to be one of the most promising and important areas of research over the next decade and beyond and rapid advances in the state of the art are anticipated. The importance of high magnetic field research has been detailed in a recent report produced by the NAS [7], which specifically called out the importance of combining magnetic fields with scattering probes. This capability will impact frontier areas of quantum materials research, including quantum critical matter, frustrated magnets, superconductors, and topological phases. The NAS report explicitly recommends expansion in the availability of modern 10-16 T cryostats as expeditiously as possible, the development of 40 T or greater pulsed magnetic fields with repetition rates of 30 seconds or less, and greater wide-bore all-superconducting magnets for steady-state fields of 40 T or greater. As discussed below, we agree with these recommendations and our strategy is consistent with their implementation.

One significant advantage of neutron scattering when compared to other, wave-vector-dependent techniques is that the elastic and inelastic cross sections for both nuclear and magnetic scattering are well understood and the experimentally observed quantities are calculable theoretically. Advancements in neutron instrumentation have improved experimental efficiency allowing large volumes of wave vector energy space to be explored. Effective extraction of scientific information from these large data sets remains a significant challenge. Theoretical methods can be used to calculate experimentally observed quantities, but direct comparison between calculation and experiment requires incorporating the influence of instrumental geometry and resolution. The development of infrastructure for such direct comparison is in progress and will leverage ORNL expertise in theory and high performance computing. This will maximize the scientific output and impact from neutron scattering instruments yielding large scientific impact across a wide range of fields.

Addressing the Needs

Implementing the advanced neutron instrumentation and sample environment equipment required for research on quantum materials will be carried out with broad input from the scientific community. In the past year input has been received from NAB, a cross cutting science workshop examining future science impacts of neutron scattering across several disciplines, and specialized science workshops ranging from the science of strong spin-orbit coupling in 4d and 5d materials to high pressure research. A meeting on quantum materials is scheduled to take place at Berkeley, California, in December 2013, to specifically examine future directions in the science of quantum materials and the roles of neutrons and x-rays in related research. An additional workshop on applications of SANS to hard condensed matter is being organized with the aid of external specialists.

Flux limitations affect most areas of neutron scattering, particularly inelastic experiments but also many diffractometers, especially those operating in polarized mode. Numerous efforts are under way to enhance the capabilities of existing instruments to allow for more efficient measurements and improved signal to noise, enabling the successful completion of more challenging experiments.

At HFIR, upgrade efforts are under way to improve signal-to-noise at the Neutron Powder Diffractometer (HB-2A) by including a large two dimensional position-sensitive detector and a radial collimator. The single-crystal diffractometer Four-Circle Diffractometer (HB-3A) is being outfitted with a new detector, better sample environment capabilities, and polarized beam options. The WAND (HB-2C) is being completely modernized in all aspects to provide a competitive continuous source instrument for rapidly mapping out scattering in significant volumes of reciprocal space. SANS instruments such as those at HFIR already play a significant role in studies of structures such as vortex and skyrmion lattices. This research will benefit from planned upgrades to General Purpose-SANS (CG-2) as well as the development of improved sample environment equipment.

The existing Magnetism Reflectometer (BL-4A) on FTS is being improved with new detectors and hardware upgrades to enable measurements over a larger dynamic range and improved off-specular scattering to resolve in-plane structures. The new CORELLI (BL-9) instrument on FTS will enable rapid energy-resolved studies of disorder via diffuse scattering and will increase in efficiency through the addition of detectors until full coverage is achieved.

Measurements on novel mesoscopic, nanoscopic, and crystal structures with important features on many length scales are well matched to STS instruments, since the enhanced cold neutron spectrum and larger interval between pulses allow for measurements covering a large range of length scales. Proposed STS instruments such as polarized SANS machines, extended range reflectometers, and high-resolution diffractometers with greatly expanded wave-vector coverage will allow for much more effective elucidation of such structures. The pulsed source combined with event mode data handling also opens up the realm of time-resolved experiments that can be applied to nonequilibrium situations.

To enable continued state-of-the-art measurements of the dynamics of materials, upgrades are also planned for the inelastic scattering instruments at HFIR. Currently, the sample tables on all of the triple axis instruments, the Fixed-Incident-Energy Triple-Axis Spectrometer (HB-1A), Polorized Triple-Axis Spectrometer (HB-1), Triple-Axis Spectrometer (HB-3), and Cold Neutron Triple-Axis Spectrometer (CTAX) (CG-4C) are being improved to enable more extensive use of heavy sample environments. Backend enhancements are planned or under way for HB-1, HB-3 and CTAX. HB-1A has an upgrade path allowing for its use as a diffractometer with energy discrimination covering a wider range of wave-vector both in and out of the horizontal scattering plane. Enhancements of the ability to use polarized neutrons at HB-1 will continue into the future, and the implementation of this capability on other triple axis spectrometers will be considered. Perhaps the most exciting long-term possibility is the construction of a world-class continuous cold neutron spectrometer at HFIR. Such an instrument would ideally span energy transfer ranges up to 30 meV with excellent Q resolution, use velocity selectors and filters to eliminate backgrounds, and have a polarized scattering option. It would also allow for the insertion of spin echo devices to achieve nanovolt energy resolution well away from Q=0, providing a capability totally complementary to inelastic instruments at FTS and STS.

The inelastic instruments at FTS are producing exciting science but still have significant possibilities for improvement. Finishing the full detector complement at CNCS (BL-5) and SEQUOIA (BL-17) will significantly increase the efficiency of experiments, and arguably also allow for an improved separation of the target measurements from background signals such as those arising from sample environment equipment. The background at CNCS will be further improved by the addition of a T_0 chopper, and utilization of neutrons further enhanced by implementing multiplexing of incident energies. At HYSPEC (BL-14B), the implementation of full polarization analysis is underway using both ^{3}He and neutron optical methods, each of which can be used under different circumstances.

Investigations of magnetic excitations in the future will require measurements with excellent resolution at low energies, with a wide range of both wave-vector and energy transfer, and the possibility of polarization analysis. For these demanding experiments the high resolution and high intensity CNCS planned for STS will provide orders of magnitude improvements over existing inelastic instruments.

The science on quantum materials that can be done across the facilities at ORNL will depend crucially on the ability to achieve needed conditions of temperature, pressure, and external fields. We are committed to improving both low and high temperature and high pressure capabilities and are taking active steps in that direction through collaborations with experts and the design, fabrication, and purchase of new equipment. As discussed above, magnetic fields are an extremely important part of the strategy. We are currently acquiring improved steady-state magnets for use in instruments across the entire existing suite and will continue to upgrade this capability as rapidly as is practically possible. Initial measurements using pulsed fields up to 30 T have been successfully carried out, and a project has been initiated to develop local capabilities for greatly improving the duty cycle and ultimately the field. ORNL will collaborate with experts in Japan and elsewhere to continue the implementation of the pulsed field strategy. Clearly, pulsed fields can be used advantageously at both FTS and STS utilizing the time structure of the beam and event mode data collection. The development of pump-probe studies combining pulsed magnetic fields with light sources or electric fields will enable unique measurements of materials under nonequilibrium conditions with applications to such new and diverse phenomena as photo-induced magnetism and the evolution of glasses subject to a time-dependent field. The high peak flux and low repetition rate of STS are ideally suited to such pump-probe measurements. Finally, we plan to form collaborations with experts at the National High Magnetic Field Laboratory to develop high-field wide-bore all superconducting magnets for steady-state neutron scattering experiments. This development may be a challenging long-term project but can pay enormous dividends. The ideal situation would be the development of a stand-alone magnet that can be used at multiple instruments but the development of a dedicated high-magnetic field beam line is also being considered. The possibility that such a beam line (or indeed stand-alone magnet) may require limitations of viewing angles means that it can be used most advantageously with wide bandwidth neutrons such as provided by STS.

Beyond experimentation, we are committed to improving the quality of science by collaborating with world leading theorists using both phenomenological and numerical methods. This includes strong coupling to local theoretical efforts including those in the Center for Accelerating Materials Modeling (CAMM), CNMS, and other parts of ORNL such as the Materials Science and Technology Division. In addition, we will work to involve leading theorists from outstanding institutions in the United States and worldwide. As one step in this direction ORNL is participating in a cooperative program with an international virtual institute (VI) on "New States of Matter and Their Excitations." The VI, which is headquartered in Germany, has started activities over the past year. A joint workshop was held in Oak Ridge in 2012, and a kickoff meeting in Berlin in April 2013. Other meetings are planned, and it is anticipated that close collaborations will be formed through medium- and-long term visits.

Finally, there are possible uses for SNS investigations into quantum matter that are useful yet complementary to neutron scattering. For example, muons (via muSR) are a sensitive probe of localized magnetic fields, in some cases arising from moments too small to be measureable with neutron scattering. Over the coming years, we will work with the community to evaluate whether it is feasible and desirable to develop a muon facility using the proton accelerator at SNS.

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Materials Synthesis and Performance

There is a long road from the discovery of fundamental scientific principles to the implementation of new concepts and materials that impact energy, technology, and the human condition. Approaches must be found to create efficiently the materials underlying new technologies, including further scientific breakthroughs in processes such as catalysis and separations. Characteristics of novel materials must be understood under relevant operating conditions, including the degradation and failure mechanisms over time in service. Appropriate interfaces must be designed that enable these new materials to work synergistically in functional assemblies. The unique capabilities of neutron scattering to reveal time-resolved and energy-dependent responses of materials in practical configurations under extreme conditions are critical to the discovery and development of new materials with direct impact on our daily lives [1].

Research in this area directly addresses two of the five Challenges for Science and the Imagination:

- How do we design and perfect atom- and energy-efficient synthesis of revolutionary new forms of matter with tailored properties?
- How do we characterize and control matter away – especially very far away – from equilibrium?

A core goal of BES research is to develop a more fundamental understanding of materials synthesis and performance by investing in advanced synthesis capabilities and by integrating user facilities with advanced computational capabilities.[1] By co-locating SNS and HFIR with the OLCF and CNMS, BES has uniquely positioned ORNL to address this goal and to help realize the next generation of advanced materials needed to maintain US global competitiveness. An objective of BES research and the president's Materials

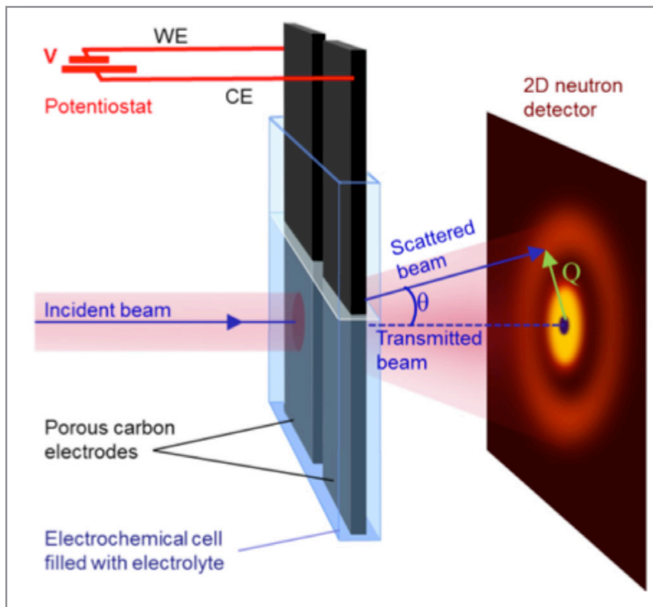

Figure 8. Measuring changes in the distribution of hydrogen atoms within a porous battery electrode, enabled by the sensitivity of neutron scattering for hydrogen, has made it possible to find where ions adsorb in electrochemical energy storage materials. This neutron-based technique opens a new route to understanding the ion adsorption process that underpins technologies including energy storage, sensing, and water desalination, and provides new insights into essential biological functions. S. Boukhalfa et al.,"Small-Angle Neutron Scattering for In Situ Probing of Ion Adsorption Inside Micropores," Angewandte Chemie International. Edition. 52, 56181-6 (2013).

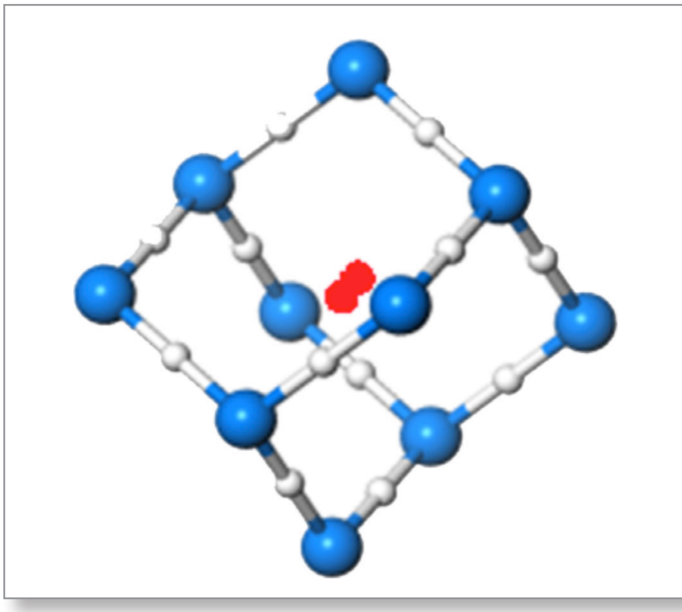

Figure 9. Hydrogen storage in ice. Combining x-ray, Raman, and neutron scattering data on the synthesis and annealing of hydrogen in amorphous ice has given new insight into the resulting structure. Simulations based on these structures indicate that ice may store up to 10 wt % hydrogen. R. Kumar et al., "Low-Pressure Synthesis and Characterization of Hyfrogen-Filled Ice," Angewandte Chemie International Edition 52 1531 (2013).

Genome Initiative is to shorten the time from discovery of new materials to characterization and ultimately to market.[2] Chemical, macromolecular and biomimetic material systems are all of importance to energy-related technologies including batteries and fuel cells, catalysis, solar energy conversion and storage, friction and lubrication, and materials and processes for energy-efficient separations.[3] New structural and functional materials are being developed for practical applications, with unique characteristics designed in through manipulation of composition, nanoscale and mesoscale structuring, and processing conditions. These diverse materials are central to every energy technology, moreover future energy technologies will place increasing demands on materials performance with respect to extremes in mechanical loading, temperature, pressure, chemical reactivity, photon or particle flux, and electric or magnetic fields [4].

Neutron scattering provides critical feedback for further improvements in synthesis and in tuning of desired properties. Several beam lines at SNS and HFIR are contributing to new understanding of metal alloys, composites, nanostructured materials, functional materials, and the interactions of materials in complex assemblies (e.g., solvation environments and electrochemical energy storage). Neutron scattering provides unique structural information for a diverse set of materials including metal hydrides, perovskites, organometallic complexes and hydrogen-bonded systems. Sensitivity to hydrogen motions, the lack of optical selection rules in neutron vibrational spectroscopy, and the penetrating power of neutrons enable in situ measurements in complex cells. This unique combination of attributes enables measurements of structure under material synthesis, and processing and service conditions, and makes neutron chemical spectroscopy an ideal tool for the study of heterogeneous catalysis. Questions concerning phase formation and transitions, stress development, and the progress of reactions and transformations can be addressed under realistic conditions with high spatial and temporal resolution. The unique sensitivity of neutrons to isotopic substitution makes it possible to understand details of local structure in complex compounds, in disordered and amorphous materials, and in solutions. New capabilities for neutron diffraction at high pressure (approaching 106 atmospheres) developed at SNS give fundamental information on the strength of chemical

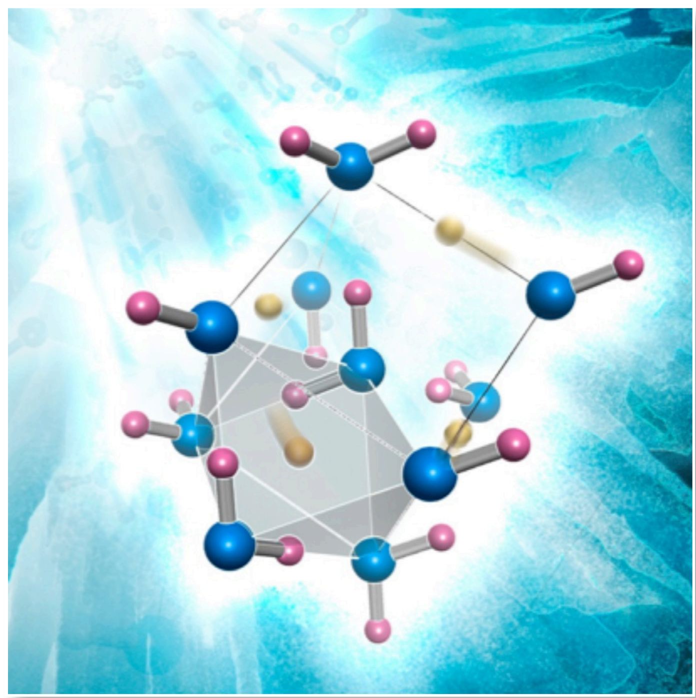

Figure 10. Neutron diffraction measurements of D_2O were extended to unprecedented pressures of 50 GPa enabling a new view of the deuterium positions in high pressure phases. Unexpectedly, this indicates substantial deuterium density at interstitial locations of the oxygen lattice which contradicts the conventional picture of hydrogen bonding in ice. M. Guthrie et al., "Neutron diffraction observations of interstitial protons in dense ice," Proceedings of the National Academy of Sciences 110, 10552 (2013). (SNS SNAP.)

bonding with applications in advanced synthesis and planetary sciences. Continuing development of neutron imaging is aimed toward making tomography and direct stress mapping widely available for applied research. Capabilities under construction for scattering measurements at ultra-small angles will bridge the gap in length scales between current SANS techniques (nanometers) and neutron imaging (microns), facilitating quantitative studies of mesoscale structures. Applying and expanding all these capabilities to answer new challenges in materials synthesis and application are primary ways for neutron scattering to contribute to materials discovery and applications.

Scientific Challenges

The primary challenge facing materials research is to achieve performance by design—creating materials tailored for specific properties, functionality, and applications. The corresponding challenge for neutron scattering is to provide experimental results that are directly relevant to understanding the formation of new materials and their resulting properties under service conditions. The power of neutron scattering to solve problems in materials design and synthesis lies in part in correlating the unique information from neutron scattering experiments with the broader range of characterization techniques to develop coherent, self-consistent models of synthesis, processing, and resulting materials performance.

Details of local composition and structure and their evolution with time and environment must be better understood to predict and control synthesis. We do not understand the complex interactions of nucleation and growth at a level that enables predictive synthesis by design. Complex reacting systems do not have the regular long-range order that is so valuable in understanding the structure and properties of crystalline materials. In many catalytically active materials, the active sites are related to defect structures rather than the regular long-range order of "perfect" crystalline materials. The strength of metals in the amorphous state can approach the theoretical limits imposed by the interatomic interactions, as compared with crystalline materials where grain boundaries and defects limit ultimate mechanical performance. The dissolution and precipitation of minerals in geological and corrosion/deposition processes in technological environments is driven by local interactions between surfaces and layers of solvent that may have very different characteristics from those in the bulk. Aggregation of macromolecules to create colloidal, gel, or film structures, and ultimately

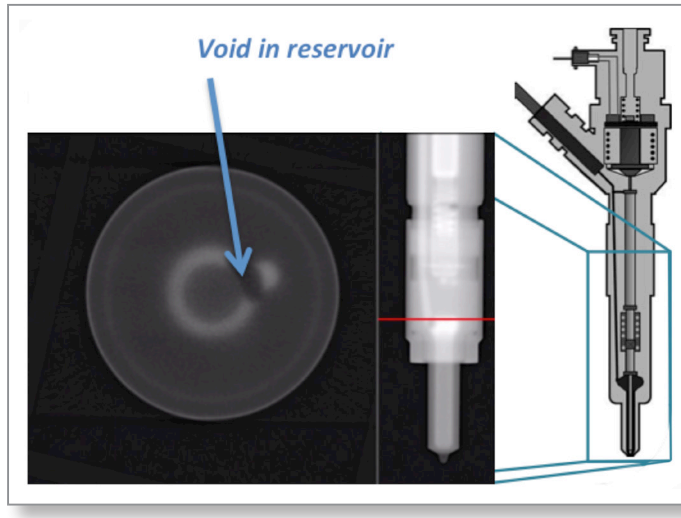

Figure 11. New details of fluid density and dynamics in commercial fuel injectors are being revealed using neutron radiography. Efforts are focused on diesel and gasoline injectors and the strong interaction of neutrons with the fuel allows for easy identification of voids in the reservoir. Future efforts will focus on internal fluid flow and understanding hydrodynamic cavitation behavior. These imaging measurements will guide and validate model currently being developed via a collaboration with ORNL and General Motors.

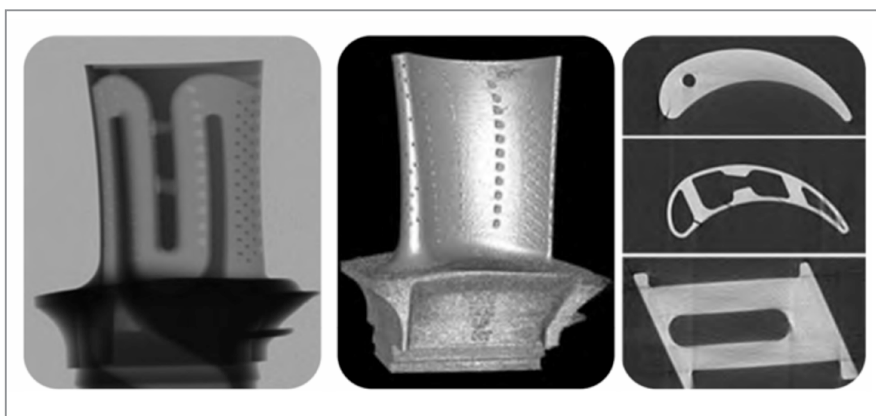

Figure 12. Radiography provides a powerful tool for the investigation of the internal structure and operations of complex machinery from manufactured parts to biosystems. The different contrast afforded by neutrons provides complimentary information to x-ray techniques. Neutron radiograph (left), volume rendered (center), and transverse slices at top, middle, and bottom (right) of turbine blade fabricated using additive manufacturing. Blade height is ~76 mm. T. Watkins et al., "Neutron Characterization for Additive Manufacturing," Advanced Materials & Processes 171, 23 (2013). (HFIR Imaging CG-1D and SNS VULCAN.)

biological structures and functions, depends on the interplay of relatively weak forces to bring reactants into alignment for the formation of complex structures. All of these processes can be driven to yield varying end products depending on the rates of reaction, which can in turn be driven by pushing systems far from equilibrium conditions. Understanding local structure and dynamics holds the key to unlocking a next level of control and design in synthesis science.

Controlling the functionality of materials depends directly on our ability to manipulate structural features and their responses to environmental changes. Incorporating functionality into structural materials (e.g., incorporating photovoltaics into paint or creating components that change shape with applied fields) is limited by our ability to control atomic and molecular alignments. We must continually develop new ways to “see” these functional interactions, within complex structures and under varying environments, to develop new synthetic approaches for enhanced functionality.

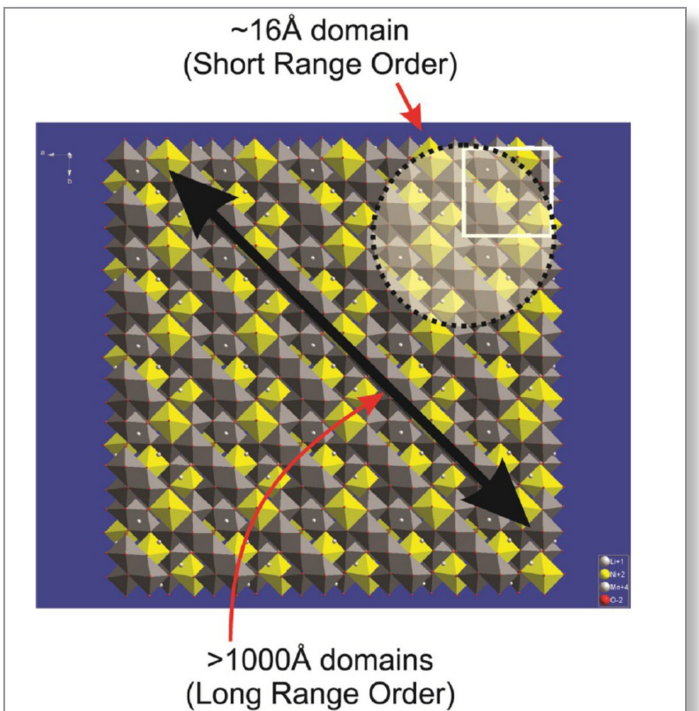

Figure 13. Multiscale order in electrical energy storage materials. Neutron diffraction studies of high-voltage doped spinel oxides show changes in cation-order domain size with annealing at elevated temperature. Dopant metals that stabilize a structure with significant cation disordering give high cycling-rate capabilities. D. W. Shin et al, “Ranges in scale of cationordered domain size in battery cathode spinel material,” Chemistry of Materials 24, 3720 (2012). (SNS POWGEN.)

Decreasing the development cycle time for adoption of new materials and processing technology in the marketplace depends on the ability to visualize structures, understand failure mechanisms, and assess the serviceability of completed components and assemblies. An improved understanding of the mechanisms and processes of failure in materials could revolutionize energy-efficient structures and systems. The time and length scales of failure range from a fluctuation leading to a local defect to the fatigue and deformation processes accruing from long-term exposure to service conditions. The ability to base failure analysis on a predictive level of fundamental science can be transformational in the conversion of newly discovered materials to useful technology.

Neutron scattering has a central role in addressing the scientific challenges of next-generation materials. Identifying gaps and opportunities and working with the scientific community to develop appropriate responses to these needs are key factors in determining our strategic direction for research in materials synthesis and performance.

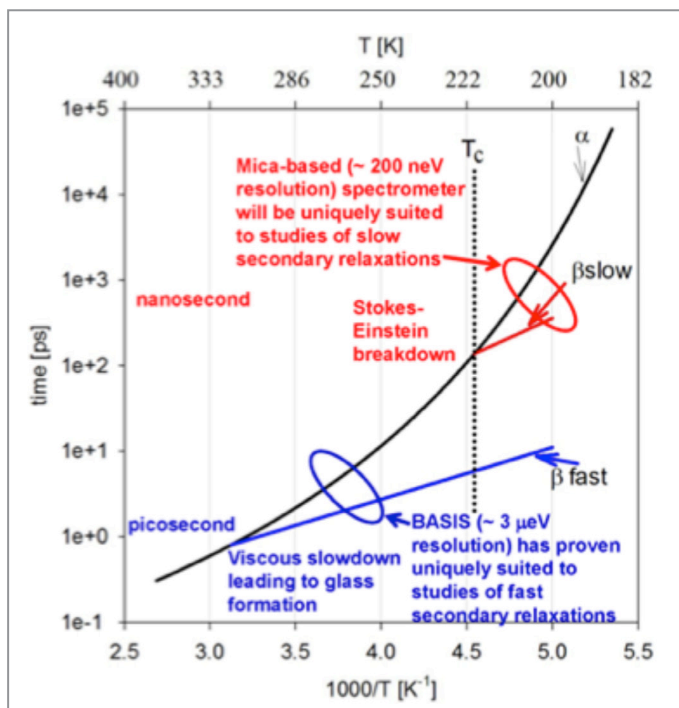

Figure 14. Expected multiple relaxation modes in glass-forming liquids that can be understood in detail with a low-energy spectrometer at STS.

Capability Gaps and Opportunities

Structural characterization historically supports materials synthesis by providing detailed information on product structure and composition. The penetrating power and elemental/isotopic sensitivity of neutron scattering coupled with the inherent timing information from a high-brightness pulsed source offer an opportunity to significantly expand capabilities to follow reactions and processes in situ. To understand more completely the actual evolution of a process, an ability to track the changes in ensembles of atoms and molecules is an important complement to ultrafast photon-based studies of changes in electronic structure. Youngs et al. [6] have recently reported time-resolved diffraction-based monitoring of a carefully crafted catalytic hydrogenation reaction. Working with catalysis researchers, there are opportunities to generalize this approach for other types of reactions (e.g., oxidative dehydration), taking advantage of the higher peak flux offered by FTS. The ability to observe operando catalytic reactions will be transformative for fundamental and applied catalysis research.

Enhanced capabilities for neutron vibrational spectroscopy (i.e., complementing infrared and Raman photon spectroscopy) are needed to further enable the study of inaccessible (e.g., opaque to photons; high-density samples) catalytic materials and processes. The commissioning in 2013 of the VISION (BL-16B) vibrational spectrometer at FTS holds the promise for improvements of more than an order of magnitude in the speed and sensitivity of chemical spectroscopy using neutrons as compared with present capabilities worldwide. It is critical to establish process-relevant experimental conditions (e.g., gas and fluid flow; variable temperature and fields) to realize the full impact of the capabilities of this instrument.

Neutron scattering offers advantages in elemental and isotopic contrast that enable addressing specific questions of composition and local structure. Usable isotopic contrast in oxygen isotopes has recently been reported [7]. The possibility of direct measurement of lithium-ion dynamics in quasielastic or inelastic scattering is being expanded. Continued development of neutron techniques offers new opportunities to interrogate structural and dynamic details in important energy technologies such as oxide fuel cells and lithium batteries. Major improvements in signal-to-noise will open new avenues for experiments previously thought to be impossible.

Limitations in our capabilities to vary internal energy in materials (e.g., through pressure and applied fields) must be overcome to better understanding bonding and structural reorganization. The high flux of SNS makes possible unique measurements of changes in structure with increasing pressure. This research is already contributing to new understanding of changing chemical bonding in water and inclusion compounds [8]. This high-pressure capability needs to be expanded to include high magnetic fields at low temperatures to open an additional dimension in the phase space for quantum materials and give a new avenue for understanding fundamental physics of materials under extreme conditions.

The ability to measure internal structure in a real component under real conditions is a key to predicting the operating properties of new materials in technological applications. A significant gap exists in current capabilities to span the important length scale from about 100 nm to tens of microns. SANS has provided important information on porosity in natural materials (e.g., samples of rock from petroleum or geothermal reservoirs) and on the details of nanoscale structure in alloys and composite materials. At longer length scales, neutron imaging is contributing quantitative information on internal structure and processes in systems ranging from engine components to next-generation battery architectures. The demand from the applied research community is for spatial resolution in imaging that bridges the gap from the current limit of about 30 μm to about 1 μm and enhanced contrast modes that would enable spatial and stress mapping in a single experiment. Realizing the promise offered by new designs for imaging capabilities at FTS could make available a new workhorse capability for applied materials research.

Resolving structural and dynamic details of water in the vicinity of solutes and surfaces is central to understanding processes ranging from corrosion and deposition to biology and life. Water is unique in its physical and chemical properties. It is as close to a universal solvent as any compound known, and those solvation properties in turn have a direct effect on the structure and dynamics of solutes. Capabilities to understand water and its solutions must be expanded to cover extended energy ranges, resolving the recently raised question of multiple dynamic relaxation modes near both hydrophilic and hydrophobic surfaces [9]. There is a tremendous opportunity to extend quasielastic scattering to nanoelectron-volt energies with the SNS STS; this could open a new door to understanding the local dynamics of hydrogen-containing solvents.

Key gaps in neutron capabilities for studies of materials synthesis and performance lie in improving resolution in direct imaging, in establishing environments for experimental studies that reflect synthesis and service conditions, and in being able to combine the unique characteristics of neutron techniques with other experimental data to advance capabilities for predictive modeling. A key theme of BES-sponsored research focuses on adding predictive capability to discovery, as evidenced by new investments in solar-fuel and electrical energy storage research hubs. Current DOE materials genome research "emphasizes the need for an experimentally proven modeling paradigm that could speed the rate of discovery of new materials and shed light on their underlying physical structure and properties" [3]. With improved instrumentation and sources, monitoring and feedback on in situ kinetic and synthetic processes will become feasible. To have the maximum scientific impact in materials by design, the unique capabilities of neutron scattering must be made available at a rate that meets the needs of synthesis science and with the transparency to contribute directly to theoretical and modeling efforts.

Addressing the Needs

Specific approaches to address these opportunities are incorporated in Neutron Sciences Directorate 5-year planning and are under active continuing discussion with the scientific community. To address the challenge of realizing atomic specificity in synthesis, we are expanding the capabilities of NOMAD (BL-1B) (the nanoscale-ordered materials diffractometer) to give it the ability to determine atomic-level structures in isotopically labeled samples with unprecedented sensitivity. To address the level of access to neutron scattering needed to support synthesis research, the POWGEN (BL-11A) (powder diffractometer) instrument is being upgraded with community input, adding detector coverage, improving signal-to-noise, and enhancing the sample environment for extreme-temperature and applied-field research. The needs of the powder diffraction community going forward were discussed in a recent workshop [10], and future workshops will focus on the need for additional high-throughput capability to support synthetic research.

Understanding materials far from equilibrium is a central driver for upgrades in progress. Sample-levitation systems based on both aerodynamic and electrostatic levitation are being commissioned on NOMAD for studies of metastable states of matter (e.g., supercooled refractory materials for temperatures beyond 2,000°C). Diamond-anvil technology for studies at extreme pressure (beyond 1 million atm) will be further developed to take advantage of the unique design capabilities of SNAP (BL-3) (the spallation neutrons and pressure diffractometer). The use of time-resolved data in following dynamic processes has been demonstrated at FTS on VULCAN (BL-7), the engineering materials diffractometer. Merging the capability for time resolution with new pump-probe capabilities (e.g., fast laser heating of small samples on NOMAD) will uniquely address questions of transient behavior in materials far from equilibrium.

DOE initiatives in applied energy research are focusing on the development of new energy-efficient manufacturing techniques for complex structures. We have shown that neutron imaging is a powerful tool for interrogating the internal structure of components and that neutron diffraction at HFIR and FTS yields key information on the residual stresses in components resulting from manufacturing and processing. The applied research community is driving the development of an instrument that will combine these capabilities. Plans and initial designs are in progress for a proposed FTS instrument to be known as VENUS, which will include capabilities for Bragg-edge imaging leading to capabilities for simultaneous imaging of structure and stress. Detectors currently being procured have spatial resolutions of a few microns, addressing a near-term need in energy storage and applied materials research.

Both the synthesis and properties of materials are dependent on their environments. Research on the BASIS quasielastic spectrometer is providing insights into the dynamics of molecular solvents near macromolecules and solid surfaces. These studies have shown that the complexity of the relaxation behavior is not fully resolved with current capabilities, and discussions with the community are planned to explore possibilities for extending quasielastic scattering to lower energies with appropriate instrumentation on STS. For higher (electron volt) energies, the research community has proposed the ELVIS spectrometer for construction at FTS. This instrument would enable studies of momentum distributions and single-particle dynamics in condensed phases. Neutron Sciences staff will work with the community to investigate further the potential scientific impact and technical specifications of ELVIS. Enhanced capabilities for magnetic fields are being implemented on the GP-SANS instrument at HFIR to address needs in fundamental physics and potential applications of magnetic fields in materials processing.

The overall optimization of instrumentation on three sources will present tremendous opportunities to expand diffraction and time-resolved research on the SNS FTS. Planning is under way for workshops aimed at exploring the possibilities for new and upgraded FTS instruments focused on emerging science challenges.

Because the ultimate scientific and technological impacts of these capabilities will depend in part on their broad accessibility, enhanced access processes tailored to community needs are being developed. A mail-in proposal process for high-throughput instruments, currently available on NOMAD and POWGEN at SNS and anticipated for the VISION spectrometer, is helping to address the need for rapid characterization to support synthesis research. Programmatic research proposals offering multi-cycle access to neutron scattering instruments will deepen the extent of collaboration among research groups involved in the preparation of new materials. We are enhancing the links between neutron scattering results and other key characterization techniques with cooperative inter-facility agreements. It is now possible to access both neutron and photon capabilities for total scattering experiments through a single peer-reviewed proposal. We are advancing ways, through access to facilities and modeling tools, for neutron scattering results to be easily and directly incorporated with data from other experimental techniques to maximize the potential for discovering and using novel functional materials.

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Soft Molecular Matter

The broad area of Soft Molecular Matter encompasses studies of polymers, surfactants, colloids, gels, glasses, composites, and even simple fluids. These materials are the quintessential mesoscale systems in that their macroscopic properties arise through a combination of interactions over several length and time scales from the nanoscale of the individual building blocks to the microscale of long chains and self-assembled arrays. This area of science is ubiquitous to the energy mission of DOE. In a recent BES report [1], polymers and soft matter were discussed in five of the six "Priority Research Directions for Mesoscale Science." These synthetic materials are composed of individual, small molecular building blocks which are covalently bound to produce new materials properties. They can be used to artificially mimic the functions of biological materials or they can be built to self-assemble in collective structures with new exciting properties.

Research in soft molecular matter directly addresses two of the five grand challenges put forth by BES [2]:

- How do we design and perfect atom- and energy-efficient synthesis of revolutionary new forms of matter with tailored properties?
- How can we master energy and information on the nanoscale to create new technologies with capabilities rivaling those of living things?

Understanding and manipulating molecular matter, both synthetic and biomimetic, and controlling the interactions between macromolecules, solvents, and hard materials represent major components of BES materials science goals. The materials characteristics of soft molecular matter depend on a delicate balance between long-range, short-range, and entropic forces yielding a wide range of tunable properties. The complex interactions of fluids near surfaces control aspects of processes ranging from dissolution and precipitation of solids to folding and binding in protein complexes. Just as the ability to measure structure at length scales from atoms to macromolecular assemblies contributes to understanding the interactions of building blocks of new materials, the ability to probe dynamic properties over wide energy (or time) scales gives insight into the energetics of these interactions and their changes with time.

Research at SNS and HFIR is discovering new knowledge on the structure and dynamics of polymers, colloids, and nanocomposites in bulk solutions, in thin films, and at interfaces. Current energy-relevant research includes studies of soft matter and soft matter composites that provide light weight structural material for reduced energy consumption in transportation. Research is also being performed in understanding active polymeric components for next-generation thin-film organic solar cells. Transport in solid-polymer electrolytes is at the heart of new battery technologies and in electricity-generating fuel cells. Examples include integrated small-angle scattering and molecular dynamics studies of multi-armed polyelectrolyte dendrimers for future optoelectronic devices and lithium transport through solid polyelectrolytes. For soft materials including new polymers, nanomaterials, environmentally responsive "smart" materials, and bio-synthetic hybrids, time-resolved neutron scattering experiments exploring structural changes at the nanoscale can be used to understand and design systems for macroscopic performance using small-angle scattering, reflectometry and spectroscopy beam lines. The Fluid Interface Reactions, Structure and Transport (FIRST) Center at ORNL, a DOE Energy Frontier Research Center, is using

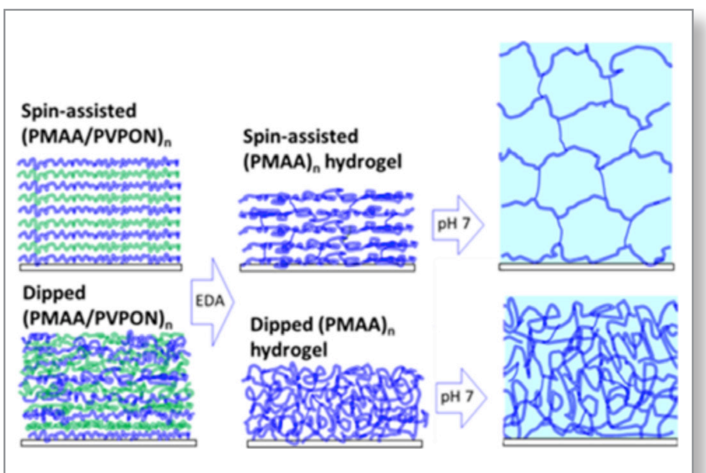

Figure 15. Hydrogels are crosslinked polymers capable of large water uptake and have applications in drug delivery, tissue engineering, and sensing. Neutron reflectometry showed how this structure dramaticaly changes the swelling properties of well-stratified hydrogels exhibiting a dramatic 10-fold increase in thickness when transitioned between pH = 5 and 7.5, unlike the 2-fold swelling observed in less-organized hydrogels. V. Kozlovskaya et al., "Tailoring Architecture of Nanothin Hydrogels: Effect of Layering on pH-Triggered Swelling," ACS Macro Letters 2, 226 (2013). (SNS Liquids Reflectometer)

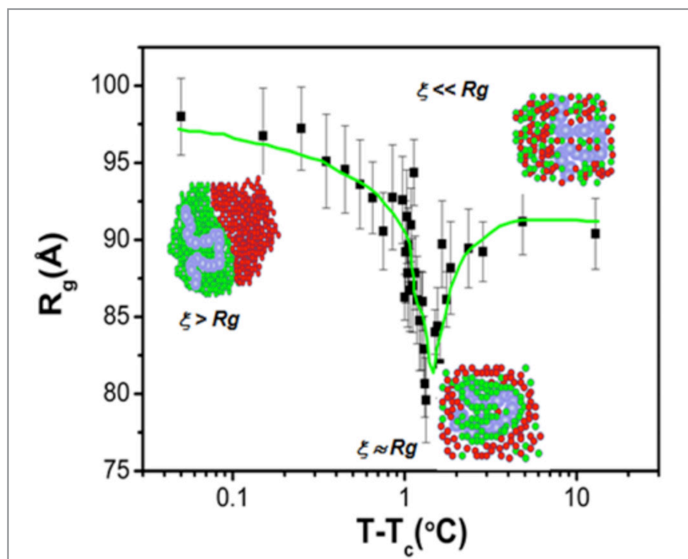

Figure 16. First experimental confirmation of the counterintuitive theoretical prediction by Nobel laureate Pierre-Gilles de Gennes that a polymer in two good solvents collapses from its swollen state and the re-swells as the solvents de-mix at Tc., the critical demixing temperature of the solvents. L. He et al.,"Partial Collapse and Reswelling of a Polymer in the Critical Demixing Region of Good Solvents," Phys. Rev. Lett. 109, 067801 (2012). (HFIR GP-SANS)

the SNS BASIS (BL-2) backscattering spectrometer to understand details of solid-liquid interfaces, while other research teams are using the same instrument to study solvation and its relation to functionality in biomolecular systems.

Scientific Challenges

The overall challenge for soft molecular matter science is to discern the competing effects of physical interactions that determine the behavior of large molecules based on the known properties of the individual building blocks. To gain a complete picture of these materials both the static structure and the dynamics must be combined to understand the interactions in the bulk material, under low-dimensional confinement, in self-organized phases of complex fluids and in composites. Some scientific challenges for the future include understanding and controlling (1) selective transport through soft membranes for fuel cells and battery electrolytes, (2) the formation and structure of porous and heterogeneous structures in polymer membranes for separation and water purification, (3) combinations of molecular and self-assembled structures to produce viable organic solar cells, (4) the addition of simple short-chained molecules to colloidal systems to make large changes in the macroscopic mechanical and aging properties, (5) the functions from biological systems that we can transfer and improve upon in synthetic materials for energy applications, (6) transport in porous media for carbon sequestration, (7) molecular and self-assembled systems for targeted delivery for self-healing materials and drug therapy, and (8) surface modification for tuned adhesion properties. In each of these areas, studies of both bulk systems and thin films are typically important since in many cases the effects of confinement play an important role in determining the final properties.

Capability Gaps and Opportunities

Addressing the main challenges in soft molecular matter will require simultaneous measurements of the structure and dynamics of materials spanning larger length scales (0.1 nm–microns) and timescales (femtoseconds–seconds) to sort out the contributions of the individual and collective subunits (atoms, molecules, aggregates). This will enable new kinetics experiments and increase the dynamic range. The mesoscale nature of soft materials also dictates that future simultaneous in situ measurements will be required under varying environmental conditions to understand their structure, function, and aging properties. This will require new instrumentation designed to provide the highest flux, but also have integrated capabilities for specialized multiprobe experiments (e.g., combining in situ optical, electrical, transport, and fluorescence measurements).

The soft matter research community has identified the need to enhance time-resolved studies of self-assembling systems, spatially-resolved studies of polymer and micellar systems, in-plane nanostructure in novel thin films and surfaces, and diffusive and collective motions in macromolecular systems. These studies are particularly critical in soft matter research because the competing interactions that determine structure and function are susceptible to kinetic control. This property enables the use of another independent variable, process rates and conditions, to profoundly affect the structure and properties of macromolecular assemblies.

Since these systems are inherently complex, modeling, simulation, and advanced theoretical tools must be integrated with experiments to produce an understanding

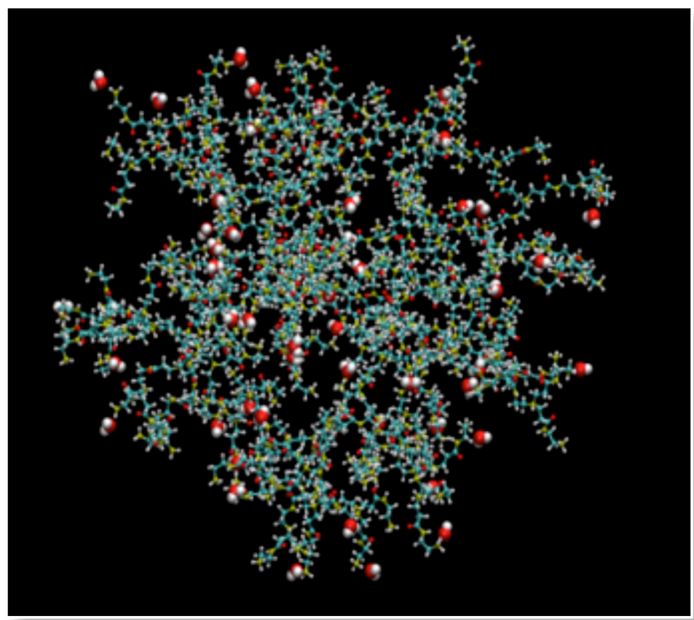

Figure 17. By combining high resolution quasielastic neutron scattering experiments and advanced theoretical and computational methods, new insight was gained concerning the dynamics of polyelectrolytes. Careful analysis of atom-by-atom computer simulations of multi-armed polyelectrolyte dendrimers dissolved in water revealed that local interactions between the polymer and only the first few nearest neighbor water molecules couples to the faster dynamics of the polyelectrolyte. B. Wu et al., "Charge-Dependent Dynamics of a Polyelectrolyte Dendrimer and its Correlation with Invasive Water," Journal of the American Chemical Society135, 5111, (2013). (SNS BASIS).

of the systems. Pure, well-characterized deuterated materials must be synthesized for any experiments to be successful in sorting characteristics attributable to any single or assembled components because small amounts of impurities can shift the delicate balance of interactions and lead to misinterpretation.

Closing these capability gaps will provide new opportunities for studies of the kinetics of soft materials and investigation of weakly scattering systems such as lithium ions and more accurate determination of the geometry of localized diffusive motions with high energy resolution. Increased high-intensity cold neutron beams will extend dynamical studies using spin echo techniques by an order of magnitude, allowing previously inaccessible correlated slow motions of domains of biological complexes to be probed for the first time. For soft materials including new polymers, nanomaterials, and smart materials such as polymer-nanoparticle and polymer-biological composites, time-resolved neutron scattering experiments exploring structural changes at the nanoscale can be used to understand and design systems for macroscopic performance. Other important new opportunities will be exploited through studying the in-plane structures of materials, from bulk heterojunctions in organic photovoltaics to stripe phases in lipid bilayers.

Addressing the Needs

The above capability gaps and opportunities were identified in the workshops "Soft Matter Current Challenges and Emerging Areas: Opportunities with Neutrons," held at ORNL in July 2011; "High Resolution Neutron Scattering to Measure Slow Dynamics," held at ORNL in March 2013; and "Future Science Impacts for Neutrons," held in June 2013 at ORNL. They will be further discussed and refined in a series of workshops scheduled with the soft matter community. Key results from these workshops are similar to those that were identified for biology, and we will address these needs with similar technology developments. However, we will also develop integrated capabilities for specialized multiprobe experiments (e.g., combining in situ optical, electrical, transport, and fluorescence measurements). Emerging Larmor precession techniques such as Spin Echo Resolved Grazing Incidence Scattering (SERGIS) or Spin Echo SANS (SESANS) are needed on new instruments at STS to push structural studies into micron length scales with real-space information on structural correlations. We will develop approaches to integrate modeling and simulation with advanced theoretical tools and experiments to produce a new understanding of soft matter systems. Development of advanced spin echo techniques would also benefit a proposed HFIR-based neutron spin echo (NSE) spectrometer optimized for low-Q and long timescales that could extend the Fourier times measured on spin echo from hundreds of microseconds to about 1 ms, pushing the limits of exploration of the slow motions of macromolecular systems.

Significant upgrades to reflectometry, small angle scattering beam lines, and imaging beam lines, as well as spin echo and backscattering beam lines, are needed to address the capability gaps identified by the soft matter research community. Examples of upgrades on existing beam lines that will enable new types of research in this area are given in the appendix. Upgrades to the small angle scattering instruments include a new sample area on EQ-SANS (BL-6) and an additional fixed, staggered set of planar detector banks on GP-SANS (CG-2) to permit coverage of a wide Q-range without moving the detector. This will enable new studies in kinetics of colloids, polymers, and surfactants to permit parametric studies of mesoscale structures. The reflectometers, Liquids Refectometer (BL-4B) and Magnetism Reflectometer (BL-4A), are in strong demand for understanding the in-plane structure of materials from bulk heterojunctions in organic photovoltaics to stripe phases in lipid bilayers. Improvements planned will provide new capabilities to perform off-specular scattering to resolve in-plane structures in thin films with features from 10 nm–20 µm. In addition, new detectors will permit both instruments to measure reflectivity over larger dynamic ranges with shorter data transfer rates. Complementing the information content in SANS experiments, the new USANS (BL-1A) instrument at FTS will enhance the length scales probed from about 100 nm to tens of microns to build an extended structural picture of soft materials from individual molecules to large complex assemblies. Investigation of weakly scattering systems such as lithium ions and more accurate determination of the geometry of localized diffusive motions with high energy resolution will be enabled on BASIS. The addition of new analyzer panels will improve the signal to noise ratio, produce 50 percent faster measurements, and broaden the Q-range at an energy resolution of 11 µeV.

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Biosciences

Biology offers an extraordinary source of molecules and inspiration for the development of new energy-related materials, devices, and processes [1]. One BES research direction is mimicking biology's energy efficient synthesis approaches to generate new, advanced materials for use under harsher, nonbiological conditions. Another is developing new bio-inspired materials that assemble autonomously and dynamically and can self-repair. In addition to inspiring new materials, understanding biology, in particular photosynthesis, can lead to new photochemistry and biochemistry approaches to photoconversion and to processes beyond primary photosynthesis, such as catalysis and biosynthesis of value-added products. Because the major repository of solar energy resides in plant cell walls, research includes the development of a greater understanding of plant and microbial cell-wall architecture at the molecular level–knowledge required for catalytic conversion of biomass into chemical fuels. Understanding biomass and its efficient conversion to fuels and other value-added products is also a major goal of industry and other government agencies, such as the DOE Office of Biology and Environmental Research (BER) and the U.S. Department of Agriculture (USDA). ORNL is host to a BER Bioenergy Research Center called the BioEnergy Science Center (BESC). Research in the biosciences directly addresses three of the five challenges for science and the imagination in the BESAC report.

- How do we design and perfect atom- and energy-efficient sythesis of revolutionary new forms of matter with tailored properties?
- How do remarkable properties of matter emerge from complex correlations of the atomic or electronic constituents, and how can we control these properties?
- How can we master energy and information on the nanoscale to create new technologies with capabilities rivaling those of living things?

Neutron scattering can probe enormous ranges of length scales and timescales, from Ångstroms to microns and picoseconds to milliseconds. Neutrons are ideal for studying multiscale phenomena intrinsic to biological processes. With no charge, they cause little radiation damage and are highly penetrating, enabling use of complex sample environments. Neutrons have energies similar to atomic motions and their spin can be coupled to magnetic fields in spin echo measurements, allowing the study of dynamic processes over picosecond to microsecond timescales. However, the most desirable property of neutrons for biology has to do with hydrogen, the most abundant element in biological systems. Photons and electrons interact with the atomic electric field. With just one electron, hydrogen is all but invisible to x-rays. Neutrons interact with nuclei, and protons have a relatively strong and negative scattering length. The isotope deuterium has an even stronger scattering length that is positive. These properties have provided neutrons with the power to determine precise information on the location and dynamics of hydrogen atoms at the atomic level through to unique information on large, multidomain complexes at longer length scales.

Biology research is an area of growth at SNS and HFIR, and neutrons are increasingly contributing to our understanding of biology and our capacity to manipulate its complexity. Many biological processes are accomplished through the concerted action of larger, multidomain proteins and multisubunit complexes. Most of these systems are not amenable to crystallization for reasons that range from their flexibility to their loosely bound or transient nature. SANS is well-suited to the study of such systems because large-scale structural information can be obtained without the need for crystallization. The use of selective isotopic labeling makes it possible to highlight the structure of a biological macromolecule within an intact, functional assembly. Large-scale assembly and disassembly processes can also be studied, and real-time experiments are possible in some situations. Neutron reflectometry is sensitive to the structures of interfaces, such as between a protein and a cellular membrane. The membrane plays a critical role in transport and signaling processes, making its understanding vital to building a holistic picture of cellular processes. Examples of other applications include using spectroscopy to characterize protein dynamics, atomic

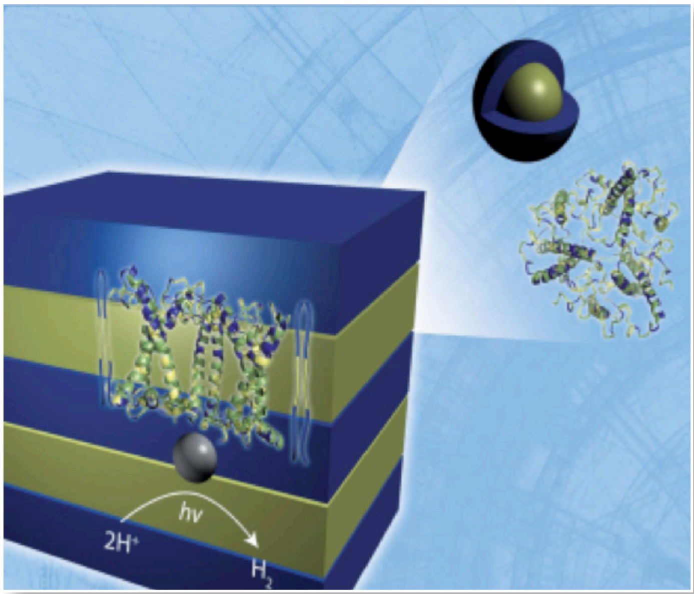

Figure 18. The large scattering contrast of hydrogen and deuterium for neutrons allowed the characterization of a photoactive biohybrid membrance that converts light into hydrogen fuel. This smart material self assembles from a synthetic block copolymer, a light harvesting complex found naturally in plants, and platinum nanoparticles. Another advantage of neutron scattering for this study is that it does not cause radiation damage. This work, as part of a DOE BES EFRC, provides a novel approach for the development of a new class of membrane-based smart materials inspired by natural photosynthetic membranes. Membrane-based systems are attractive for photosynthetic systems because their architectures optimized for the assembly of interacting components. M.B. Cardoso et al., "Supramolecular Assembly of Artificial Photoconversion Units," Energy & Environmental Science 4, 181(2011). (Bio-SANS at HFIR)

resolution crystallography to guide the design of new drugs, and using small angle scattering to characterize biological membranes.

This is a time of unprecedented opportunity for using neutrons in biomedical research. NSF- and NIH-funded researchers are using neutron scattering to contribute to our knowledge about the delivery of drugs and to understanding of the action of anesthetics, understanding the origins of diseases such as neurodegenerative Huntington's and Alzheimer's, viral and bacterial infection, and toxin decontamination. In biotechnology and biomaterials, neutron scattering is contributing to the rational design of new industrial enzymes and new bio-inspired materials and sensors. In BER research, SNS and HFIR neutron-scattering capabilities are being combined with OLCF molecular simulation capabilities to image changes in biomass morphology as it is converted into fermentable sugars and the subsequent enzymatic conversion of those sugars into fuels and other products.

Scientific Challenges

Several agencies sponsoring science at SNS and HFIR have commissioned reports that have identified the greatest scientific challenges in biology that we will face over the next few decades and the new strategies and innovative tools required to address them [2–4]. In the reports commissioned by DOE, NIH, NSF and NAS, common themes arise of a need to understand and predict the behavior of complex biological systems across length scales and timescales using multidisciplinary approaches that exploit recent technological and scientific advances. Indeed, the challenge of understanding and predicting the behavior of complex biological systems drives progress in BES biomaterials research [1]. Recently, a BES-sponsored workshop report [5] recognized that biology displays many compelling features of mesoscale science and emergent systems. The report said, "Imagine the realization of biologically inspired complexity and functionality with inorganic earth-abundant materials to transform energy conversion, transmission, and storage."

The challenge of understanding the interplay between structure and dynamics that gives rise to scale-spanning biological functions is immense, and it requires the application of multiple experimental and computational techniques to understand even the most basic processes. Biological systems rely on a fine balance between regular structure (order) and dynamics (motion) to carry out highly regulated processes. Molecular events span times from under a picosecond (10^{-12} s), the time it takes for energy transfer in photosynthesis, to more than a gigasecond (10^{9} s), the lifespan of a multicellular organism. The length scales in living organisms range from less than an Ångstrom (10^{-10} m, the length of a chemical bond), to multicellular organisms larger than 10 m. The interpretation and integration of the resulting spatiotemporal data with other biological, biochemical, and biophysical work to create scientific understanding requires the application of advanced theory, modeling, and simulation and represents an interface between the biological and physical sciences at the forefront of research. Better integration within biology, and closer collaboration with physical, computational, and earth scientists; mathematicians; and engineers; has been recommended as a "new biology" [3]. This approach will be essential for advancing the new emerging field of synthetic biology that offers the opportunity to redesign life at the molecular level. Synthetic biology is a cross cutting field at the nexus of molecular, cell, and systems biology that impacts everything from biomedicine to bioenergy.

Capability Gaps and Opportunities

As we move toward studying more complex biological systems there is a need for new experimental capabilities for characterizing biological systems simultaneously over great length scales and timescales, with better time-resolution, and beyond the current limitations imposed by sample size. Imagine following changes in a real biological system using neutron scattering with a time resolution of less than a millisecond over length scales and dynamic timescales ranging from the atomistic (~1–10 Å/~10–100 ps) to those involving assemblies of macromolecules (~100–1,000 Å/~1–10 ns). Closing this gap would open up new opportunities for studying receptors and synthase complexes; signaling pathways and the structure and dynamics of their multicomponent complexes; and the imaging of complete functioning cells and microbes, higher organisms, and organs. New classes of time-resolved experiments would be possible for following simultaneous structure evolution over large length scales; exploring disease-associated amyloid plaque growth; and studying the functioning assemblies associated with DNA regulation and repair, molecular machines, viral infection, and drug delivery systems.

One example of such a complex biological system is nature's most efficient device for gathering light, the chlorosome. Chlorosomes resemble the dipole antennas humans have engineered for optimizing reception of radio waves, but with length scales commensurate with the wavelength of visible light. It is currently unknown how the high efficiency of light absorption by natural antennas and its subsequent conversion to the quantum states of pigments and localization to a reaction center works. It appears likely that coherent quantum states of the arrangement of pigments in the photosynthetic antenna play a role in this process because transport through simple absorption/emission processes along a chain of pigment molecules is unable to explain the high efficiency. Neutron scattering provides unique capabilities to study these structures and their response to photo-stimulation. To close capability gaps in chlorosome research, there is a need for improved scattering instrumentation that allows simultaneous measurement over length scales from the micrometer range (light wavelength) to the reaction centers (biocatalysts 1–10 nm scale), pigments (~1 nm scale) and beyond to the atomic scale to reveal details of the biochemical processes that are powered by the light antenna. There is also a need to perform such measurements with high time resolution and in situ, (i.e., in response to photo-stimulation and during the kinetics of light-driven reactions.) Importantly, a deeper understanding of these processes holds the promise of more efficient use of solar energy not only for the generation of electricity and fuel but for a range of higher value-added compounds and materials by coupling respective designed catalysts (biological enzymes, reaction, centers or their synthetic analogues) to efficient light-gathering antennas (whether natural or bio-inspired mesoscale devices).

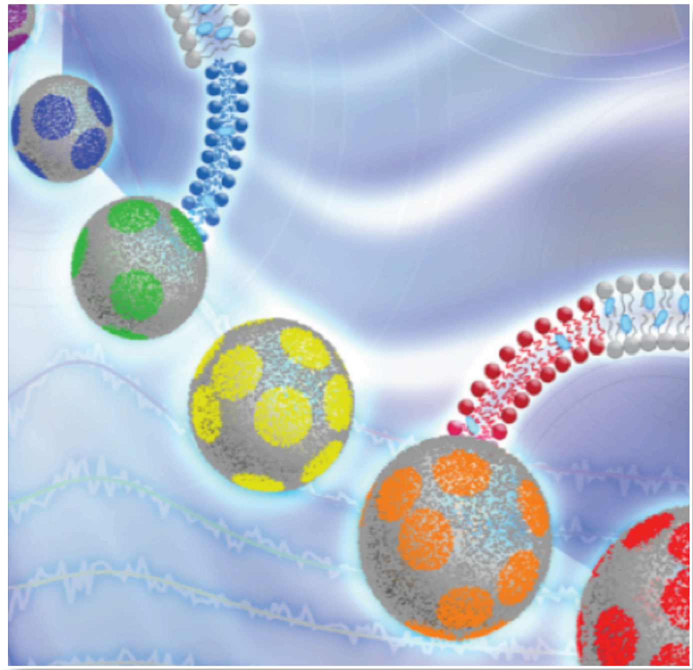

Figure 19. Plasma membrane microdomains ("rafts") occur in prokaryotic and eukaryotic cells. They are thought to play a vital role in signal transduction, protein trafficking, and viral pathogenesis. Using small angle neutron scattering (SANS) combined with selective lipid deuteration and contrast matching, domain size and thickness were measured in biomimetic membranes, without the addition of extrinsic probe molecules commonly required with other techniques (e.g., fluorescence). Domain size was found to depend on the thickness mismatch between the raft and its surrounding sea. Precise SANS measurements of raft size and thickness will help refine existing theory and lead to an understanding of raft formation and dissolution in cells. This represents a demonstration of an approach for characterizing the Membranes, organelles, and walls of whole cells. F.A. Heberle et al., "Bilayer Thickness Mismatch Controls Domain Size in Model Membranes," Journal of the American Chemical Society 135, 6853(2013). (HFIR, Bio-SANS).

New methods are required to enable the study of in-plane structures at biological membranes and interfaces from 10 to 1,000 nm, allowing investigation of aggregation processes associated with disease, exploration of the action of anesthetics, and development of membrane platforms that could emulate biological processes such as transport and photosynthesis. Imagine mapping out the regulation and transport of molecules through protein channels across biological membranes. This would represent a revolutionary new capability for biology, and the impact for the development of new therapeutics and biomimetic systems would be significant.

A limitation to the application of neutron crystallography and spectroscopy to understanding biocatalysis is the large sample size required. Smaller beam sizes and higher cold neutron fluxes will allow for much smaller samples of more complex systems to be studied, thus allowing high-resolution neutron crystallography to be applied to characterize membrane proteins and their function for the first time. Spanning this sample-size capability gap would provide new opportunities for using neutron crystallography in the development of improved drugs against multi-resistant viruses and bacteria, understanding enzyme mechanisms and the regulation of metabolic pathways for synthetic biology. Neutron spectroscopy could interrogate both enzymes and bio-inspired catalysts that hydrolyze biomass or convert products to advanced biofuels through hydrogenation or syngas conversion.

Biological fibers were the initial driving force for the development of synchrotron sources for structural biology. Currently there is no neutron instrument optimized for studying fibers or biological tissues. A new facility for neutron membrane and fiber diffraction will close this capability gap in the United States. This instrument will require sample environments with relative humidity (RH) control, for studies of collagen, skin and bone, muscle, filamentous viruses, nucleic acids such as DNA, amyloid systems, and various polysaccharides in their natural fibrous state.

The key to integrating the information obtained from neutron scattering on complex systems will be the development and use of computer simulation techniques. Significant progress has been made in the timescales and length scales accessible to molecular dynamics simulation, and it is now common to probe systems of ~10^5 atoms on timescales of ~100 ns. This increase in scope has allowed many biological processes to be characterized because the length scales accessible to molecular dynamics interpretation could be extended. However, the challenge is extrapolation of current performance to the exascale which will, in principle, enable computer simulation

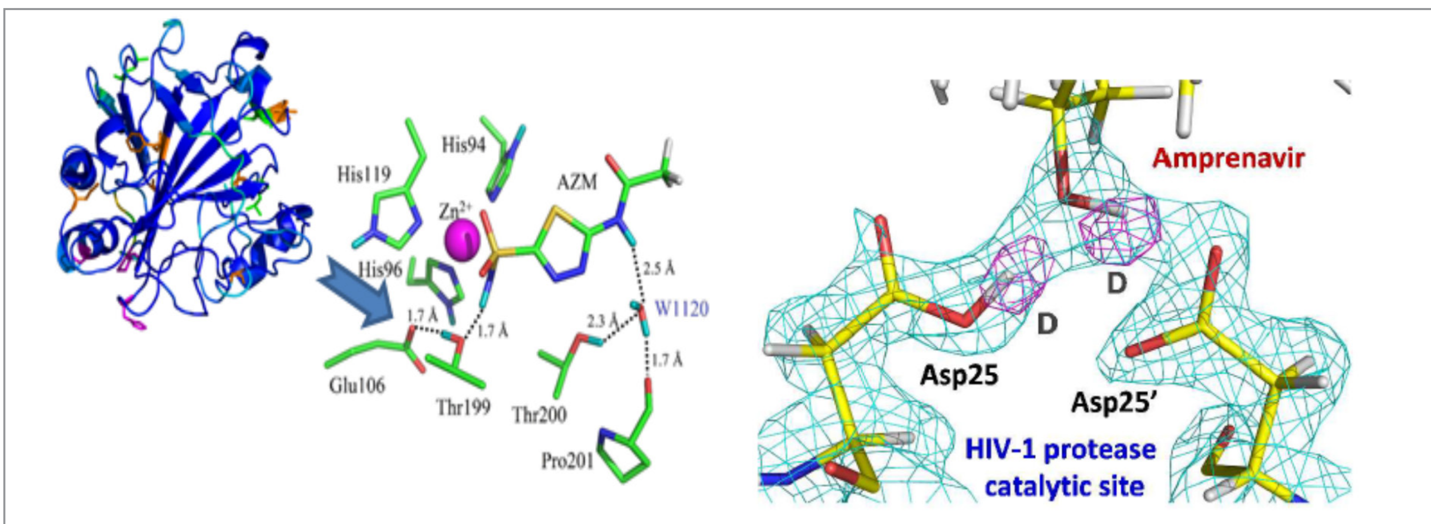

Figure 20. The sensitivity of neutrons to hydrogen and deuterium makes neutron crystallography one of the only techniques that can be used to reveal the position of hydrogen atom in protein-drug complexes. Recent results could guide the development of new drugs for human carbonic anhydrase (left) and HIV protease (right). New beamlines MANDI and TOPAZ at the SNS FTS, and IMAGINE at HFIR, will quadruple the number of beam lines suitable for neutron macromolecular crystallography in the United States. Capabilities will be extended to larger and more complex biological systems at the STS. S. Z. Fisher et al., "Neutron Diffraction of Acetazolamide-Bound Human Carbonic Anhydrase II Reveals Atomic Details of Drug Binding, "Journal of the American Chemical Society 134, 14762 (2012), and I. T. Weber et al., "Joint X-ray/neutron crystallographic study of HIV-1 protease with clinical inhibitor amprenavir – insights for drug design," Journal of Medicinal Chemistry 56, 5631(2013).

of the Newtonian molecular dynamics of systems of ~10^{10} explicit interacting atoms (i.e., about the number of atoms in a living cell). This advance alone may lead to a revolution in the energy biosciences, allowing the detailed simulation analysis of microbial:biomass and enzyme:biomass interactions critical to second-generation biofuel production.

The above capability gaps and opportunities were identified in a "Frontiers in Structural Biology" workshop that was held in May 2013, at ORNL and in a "Future Science Impacts for Neutrons" that was held in June 2013. They will be further discussed and refined in a series of workshops with the biology scientific community, the first of which will be held in San Diego, California, in January 2014.

Addressing the Needs

We will address the need to measure simultaneously over greater length scales by building additional wide angle detector banks for the small angle scattering instruments Bio-SANS (CG-3) and GP-SANS (CG-2) beam lines at HFIR and the reflectometers, Liquids Refectometer (BL-4B) and Magnetism Reflectometer (BL-4A) at FTS by completing construction of a new Ultra-Small Angle Neutron Scattering (USANS) (BL-1A) instrument at FTS and by developing new types of combined wide and small angle instruments (SANS/WANS), USANS/WANS, and reflectometer beam lines at STS. With these developments, we will extend the length scales that can simultaneously be accessed by orders of magnitude compared to existing beam lines at FTS and HFIR. The enhanced long wavelength neutron flux at STS also opens up the exciting possibility of using polarized neutrons with Larmor precession (spin echo) techniques that access larger length scales or provide greater measurement precision, as discussed previously for soft molecular matter. The increased peak brightness of long wavelength neutrons at STS will also allow smaller beam sizes to be used. This opens up the possibility of using grazing incidence techniques, originally developed at synchrotron photon sources, to study in plane structures at surfaces and interfaces.

One very common and large capability gap for all instruments at FTS and HFIR that are used for biology, in particular the atomic resolution single crystal diffractometers, MANDI (BL-11B), TOPAZ (BL-12) and IMAGINE (CG-4D), is the weak flux of available neutron beams, which results in limited signal-to-noise ratios and a requirement for large samples, or long data collection times for small samples. This gap will be closed by increasing neutron flux, increasing detector coverage by adding more detectors to maximize data collection efficiency, using longer wavelength neutrons to maximize reflectivity, or preparing deuterated samples to increase the scattering power of samples. Another approach is to explore innovative approaches to reducing instrument background and improving signal-to-noise ratios. Existing instruments will be upgraded to have a complete complement of detectors as discussed in Appendix B. Further, we will develop novel moderators and focusing neutron optics devices that will increase flux by at least an order of magnitude and produce focused beams for biological reflectometry and crystallography on large complexes at STS and for time-resolved studies on beam lines across the ORNL neutron complex. There is a need for a flexible diffractometer for studying partially ordered biological systems and tissues such as fibers and membranes. Such an instrument will be best located at STS or the cold source at HFIR. Enhancing neutron flux and opening up simultaneous access to the nanoscale and mesoscale will enable time-resolved studies with new opportunities for pulsed and pump probe experiments.

The development of inelastic techniques for probing biological dynamics is expected to be an important area of growth for biology over the future and will provide key knowledge required for designing new biomolecules important for biomedical and bioenergy applications. However, neutron spectrometers have common needs that greatly limit their broad application. In particular there are needs for accessing longer dynamic time scales, increasing data collection rates, and allowing the use of smaller samples. These gaps will be overcome by enhancing some of the basic instrument components and, more importantly, by relocating or building new instruments on neutron sources with better matched spectra of cold neutrons. Specifically, construction of an NSE instrument at HFIR will enhance its performance by over an order of magnitude in some configurations. NSE at SNS is designed primarily for soft-matter research, although its capabilities also make it potentially useful for all fields of modern condensed matter physics, materials science, and biophysics. This instrument is especially suited for analyzing slow dynamical processes and thereby unraveling molecular motions and mobilities at nanoscopic and mesoscopic levels. A backscattering spectrometer will be built at STS to extend reach to longer dynamic time domains. A backscattering spectrometer can be used to probe dynamic processes in various systems on the picosecond to nanosecond time scale. It is well suited for probing diffusive and relaxational motions but can also be effectively used for studying some types of collective excitations in condensed matter. Both of these upgrades will open up new avenues of scientific research in energy-relevant biomaterials.

Deuterium-labeling and high performance computing are not easily used by most biomedical researchers and currently are not readily available to support neutron scattering. Our strategy is to integrate neutron scattering with powerful high performance computers operated by ORNL and the University of Tennessee, and a deuterium-labeling laboratory operated by the Center for Structural Molecular Biology (CSMB) located at SNS. The best labeling strategy will be guided by computer calculations of neutron scattering from different labeling permutations. Further, simulations of structural and dynamic changes in the complex will guide the choice of neutron instrument configuration most likely to detect those changes. The dynamic nature of complexes is fundamental to their biological function and yet it is one of the greatest challenges to the structural biology community. To understand these biological switches and machines requires exploring in parallel multiple length scales and timescales. Neutron scattering data, along with other experimental data, will be used to steer construction and simulation of a multiscale realistic physical model of complex assembly and disassembly during regulation and function.

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NEW AND UPGRADED CAPABILITIES

Enabling Technologies

The current instrument suites at SNS FTS and HFIR cover the broad ranges of length, time and energy scales typical of neutron scattering facilities. Since 2007, the results from experiments on these instruments have been producing a rapidly increasing number of high impact publications. The growth trend is expected to continue as newer instruments mature and develop a cadre of experienced users; four additional instruments enter the user program; the operating power of SNS reaches its design goal of 1.4 MW; and additional operating cycles are added at HFIR. Continued growth in science impact will rely on using current beam lines in more innovative ways, upgrading and building out empty beam lines and adding a STS that complements the existing ORNL neutron sources. The low-repetition rate and long-wavelength optimization of STS will fill a key need for studies of complex materials, fitting between the capabilities of SNS FTS and HFIR, as discussed in Appendix A. With three complementary sources, ORNL will have an unprecedented opportunity to match neutron scattering techniques, instrument selection and instrument design to the source characteristics that deliver the highest performance. Instrument upgrade plans focus on scientific capability while minimizing disruption of ongoing user operations. Improvements in the current neutron sources such as better moderator optimization and raising the operating power of SNS benefit large numbers of beam lines, increasing the capacity for science and enabling more challenging or comprehensive measurements. Individual instrument upgrades will often require development of new technologies such as higher performing detectors and routine implementation of developed technologies such as ^{3}He polarization cells.

Developments in a number of supporting technologies are required to ensure the continued growth in science impact of the ORNL neutron sources. The overarching goal is to make better use of available neutrons. A hierarchy of activities and development strategies is illustrated in the pyramid diagram shown in Figure 21. A base of on-going, sometimes incremental, improvements must be maintained in order to improve the efficiency with which neutrons are used. Examples include SNS target lifetime extension, expanding the suite of reliable sample environment capabilities, and installing new components control systems that make instruments easier to use. Gains in these areas improve the throughput of the neutron scattering instruments.

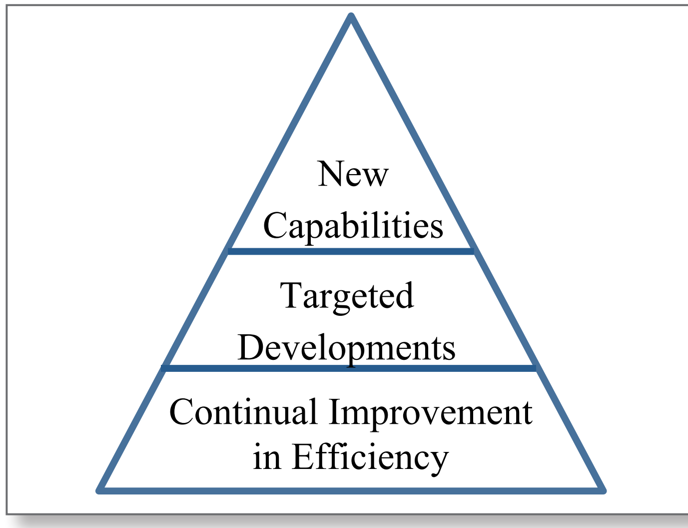


Figure 21. The hierarchy of activities in the development of enabling technologies.

A sustained effort targeted to specific outcomes where the scientific impact is clear and predictable is the prime focus of the development groups. Targeted improvements can be multiplied to provide the gain in performance required to exploit new scientific opportunities such as kinetic studies of transient phenomena in energy related materials. Many of these activities are grounded in core capabilities that have been developed within ORNL such as ^{3}He polarization cells. Others include external partnerships with other neutron centers (e.g. MANTID development in collaboration with ISIS) and collaborations with the private sector leveraging DOE investment in the Small Business Innovation Research (SBIR) Small Business Technology Transfer (STTR) program.

At the top of the pyramid in Figure 21 are visionary and more speculative developments, some of which will lead to new capabilities that extend the length and time scales that can be accessed by neutron scattering or provide fundamentally new types of information. These areas include development of Larmor precession techniques that access larger length scales or provide greater measurement precision, adaptive optics systems that focus neutron beams to ever smaller sample areas and improve signal-to-noise, the development of new multiplexing techniques, and the implementation of unique sample environments such as high-Tc superconducting magnets. Important strategies for these types of development include leveraging ORNL competencies such as leadership in computational sciences and nanoscale fabrication, collaboration with research groups at universities and maintaining a network of interactions with other facilities and groups engaged in similar research and development efforts.

Detector Development

Neutron detectors are an absolutely critical technology for the success of the science programs at HFIR and SNS. Increasing the count rate of an instrument by adding detectors is perhaps the most cost-effective way to improve the over all science output of the instrument. Planned bean line detector upgrades are discussed in Appendix B. Low-cost, large-area, modest resolution, high counting-efficiency detectors are also required as replacements for ^{3}He tube detectors as ^{3}He becomes more scarce. ORNL is a partner in the International Collaboration on Neutron Detector Development (ICND) (http://icnd.org) which is seeking alternative technologies for ^{3}He detectors. The ORNL contribution involves further development of Wave-Length Shifting Fiber detectors with improved counting efficiencies, better spatial resolutions, and lower cost. These developments will improve the efficiency and lower the cost of detector build outs for SNS powder diffractometers.

In addition to the ICND collaboration, ORNL is collaborating with a number of small private U.S. companies and several university-based researchers to test and develop detector technologies. These collaborations typically leverage DOE and other agency investments in ^{3}He replacement detectors programs.

Novel detector technologies developed over the next 10 years are likely to be transformational for the design and performance of several neutron scattering instruments. For example, the development of very-high spatial resolution detectors (1 micron) with excellent timing characteristics will bring neutron real-space imaging down to the maximum length scales currently accessible with diffraction instruments, eliminating the gap in length scales that can be accessed by neutrons. This resolution is one of the goals of the proposed SNS VENUS (BL-10) imaging station. These technologies are being effectively developed outside of ORNL and we collaborate in their testing. Neutron detectors are typically either planar in geometry or cylindrically curved. Detectors which can be curved spherically will both reduce parallax and allow the effective implementation of methods such as the Larmor-precession technique MIEZE (Modulated Intensity by Zero Effort). ORNL is pursuing a gas-amplification detector which holds promise for both this application and for meeting the large-area, high resolution detector needs of SNS reflectometers.

Neutron Optics

Advanced modeling tools and new technologies have enabled dramatic advances in the design of neutron optical devices. The ability to manipulate the angular and spatial characteristics of a neutron beam and match it to the demands of the sample (size, geometry) and the instrument have progressed from using simple focusing devices like guide “trumpets” to large, precisely curved, elliptical mirrors. As an example, the beam delivery system of HFIR IMAGINE (CG-4D) instrument provides a six-fold gain in neutron flux on sample compared to a conventional optical system. Reflective mirror devices are maximally effective for the long-wavelength neutrons that STS will deliver. Neutron beam delivery systems using elliptical mirrors will allow us to achieve maximum benefit from the small, high-brightness moderators envisaged for the STS. The development of adaptive optics systems with fine control over segmented or continuous elements may allow finely focused neutron beams (~10 microns) required for the study of small samples such as those intrinsic to ultra-high pressure measurements. Compact focusing devices will provide similar gains for some current instruments where smaller samples and transient phenomena are studied. ORNL will collaborate internally and externally in the development of these devices.

Technique Development

Many of the most innovative recent advances in neutron techniques involve the use of polarized neutrons either as a probe of magnetic phenomena (e.g. polarized neutron imaging of magnetic domains) or via spin precession to access long length or slow time scales. ORNL will continue to develop and commission spin-polarized ^{3}He cells to provide polarized neutrons and polarization analysis on existing beam lines at both SNS and HFIR for magnetic scattering applications. Full deployment requires sample environment development that combines very low temperatures with an x,y,z magnet that is integrated with beam transport elements. New capabilities achieved using spin precession techniques reach the length and time scales relevant to mesoscale science. The limits of these techniques and the implications of deploying them at a spallation source that uses a broad band of cold neutron wavelengths must be explored. ORNL has a strong external partnership in this area and intends to develop its expertise by building a cold, polarized test beam line at HFIR.

The high peak neutron flux per pulse of SNS and time-event data collection are the essential elements that allow us to probe the structure and dynamics of materials in non-equilibrium or short-lived states and to investigate transient phenomena. Both NOMAD (BL-1B) and VULCAN (BL-7) have demonstrated the ability to collect data in a "single-shot" mode using the intrinsic 60 Hz repetition rate of the accelerator to capture a complete data set in 13.7 msec. Phenomena that evolve on slower time scales allow even more detailed measurements with higher statistical accuracy and the use of smaller samples by summing data from multiple accelerator pulses. For samples that can be reproducibly cycled by the application of an external pump such as mechanical loading, light, or other applied fields, probing transient behavior on even shorter time scales is possible. By controlling the timing of the applied pump relative to the neutron pulse, the time-event data collection technique allows the data to be organized into time-bins as short as 10–100 μsec. A standardized electronic interface to the data acquisition system, data reduction tools through the MANTID project, and specialized sample environments are needed to realize this capability.

Sample Environment

A great advantage of neutrons is their ability to penetrate the barriers needed to maintain the scattering sample in a particular thermophysical environment. As science goals evolve, different equipment will be needed to explore samples under relevant conditions, i.e., in situ and in operando. SNS time-event data collection mode and high peak flux are well suited to these studies but require the development of robust, user-friendly interfaces that are flexible enough to keep pace with rapidly evolving scientific directions. An important baseline goal is to ensure that the suite of "standard" environments including high and low temperature, magnetic fields and moderately high pressure is widely available and functions efficiently and seamlessly with the neutron instruments.

Targeted developments can be identified across four thematic areas that encompass the majority of sample environment equipment deployed at neutron facilities: magnetic fields, low & high temperatures, high pressure, and highly specialized apparatus for soft matter. The high peak flux of SNS favors the use of pulsed, very high-field magnets (30 to 40 T and beyond) that can be placed in existing beam lines. Routine use of this technology relies on increasing the duty factor of existing magnets and modifying the coil design to allow better neutron beam access to the sample. The study of materials at highest temperatures requires laser-heated samples, levitated in the neutron beam. In partnership with external researchers, ORNL is developing the expertise to operate and support both aerodynamic and electrostatic levitators for routine use on both elastic and inelastic beam lines. The ORNL collaboration with world leaders in high-pressure techniques has already achieved a record pressure for neutron studies of 98 GPa using a diamond anvil cell. Routine access to pressure coupled with development of high sample temperature capabilities will establish new frontiers for the application of neutron scattering in the geosciences. The study of soft matter (including biology) requires apparatus that tends to be highly specialized to particular classes of instruments such as SANS and reflectometers. This category includes Langmuir troughs, controlled humidity cells, environment control chambers, controlled light illumination, flow and electrochemical cells, and in situ bioreactors. Development is typically iterative, requiring specialized skill sets and the closest integration of science and technical requirements.

SNS has effectively used time-event data collection mode to further our understanding of transient and non-equilibrium phenomena, such as the structural evolution of batteries during charge/discharge cycling, and the response of magnetic systems to large pulsed magnetic fields. Continued development of sources and instrumentation at FTS and STS that enable high peak flux, in combination with event mode data acquisition and the development of new sample environments will allow for expansion of in situ, in operando, and pump-probe studies in the time domain as outlined above.

STS presents a set of new opportunities in the integration of sample environment equipment with instrument design. As an example, advances in high field magnet design and technologies could couple a very high field, hybrid magnet (25 T superconducting, >15 T resistive) with a scattering instrument optimized to use the high-brightness, coupled moderators at STS. This instrument would create the world's premier facility for neutron scattering at the highest continuous magnetic fields and provide unique insight into collective behavior in solids, advancing our ability to predict and control magnetic and superconducting materials. The very high peak flux of the STS long-wavelength, coupled moderators will enable fast kinetic measurements that require the development of apparatus that has not been commonly deployed on neutron beam lines. One example is monitoring the in situ growth and development of thin films by integrating a sputtering machine on a reflectometry beam line. Studies of the evolution of magnetic ordering and its dependence on film deposition parameters and thickness will promote the development of alternatives to rare earth magnets. ORNL is partnering in this area with researchers supported by the Critical Materials Institute at Ames Laboratory, as well as with experts at other U.S. facilities and universities.

Support Laboratories

The most efficient and successful use of neutron beam time requires user support laboratories for safe sample preparation, characterization, and handling. Both central support facilities and in some cases satellite installations co-located with beam lines are required. For example, the small angle neutron scattering instrument Bio-SANS (CG-3) at HFIR sits next to a small angle X-ray scattering beam line and a biology laboratory. ORNL will continue to develop and expand its laboratory facilities to support growing user and programmatic research in our science priority areas. These will provide capabilities that are complementary to and enhance the impact of neutron scattering measurements, such as x-ray diffraction, and thermodynamic and transport property measurements. In addition, CNMS is co-located with SNS and maintains a suite of routine and specialized materials synthesis and characterization tools that can be accessed by users of both facilities. Our strategy is to optimize the core suite of SNS laboratory capabilities with consideration for techniques that are already well-supported at CNMS.

Active and growing sample preparation and characterization laboratories for biology and soft matter are operating at SNS with contributing sponsorship from other organizations (e.g., DOE BER and NIH). Deuterium-labeling is of fundamental importance for biological and soft matter neutron scattering. We provide access to deuterium-labeling facilities to ensure the most innovative and efficient use of neutron scattering. These facilities will provide benefits not just in higher quality and throughput of routine experiments, but also in new, more sophisticated and more powerful approaches for solving complex problems through the development of selective deuteration strategies. The ORNL deuteration facility at SNS is envisioned to develop into a repository and distributor of the expertise required for routine and custom production of deuterium-labeled molecules for researchers. Complementary specific expertise in deuteration of small molecule building blocks, monomers, and polymers for neutron and NMR studies is available through the CNMS.

To optimize scientific output it is often necessary to combine neutron scattering experiments with other complementary characterization methods. Typically for quantum materials research the most important of these involve x-ray scattering, bulk and thermophysical measurements and transport measurements. In Europe, it has been found that making these techniques available to neutron users and local staff has had great benefit for the quality and publication throughput of the neutron facilities, with the Helmholtz Zentrum Berlin being a prominent example. To address these needs, we have plans to equip laboratories within NScD that will be available to both users and staff scientists. The facilities will include a single crystal x-ray diffractometer with low temperature capability which will be added to the existing x-ray laboratory, and additional laboratories specializing in bulk magnetic characterization and some sample synthesis.

Data Analysis and Visualization

The scientific impact of data collected in a neutron scattering experiment is only realized in its analysis, interpretation (modeling), and ultimately its communication and publication. ORNL is targeting three areas to improve data analysis and visualization. First, scientific productivity and impact can be enhanced by lowering barriers to scientific interpretation. ORNL took a step in 2010 by partnering with the ISIS neutron scattering facility in England on the joint development of the MANTID data reduction and analysis software package. Further development of MANTID is expected to provide foundational support for data reduction and analysis. Second, efficiencies in the use of beam time can be achieved as visualization and analysis of reduced data approaches near real time availability, providing feedback during the performance of an experiment. This is the goal of the ADARA (Accelerating Data Acquisition Reduction and Analysis) Project. ADARA combines resources from the ORNL Computing and Computational Sciences Directorate (CCSD) and NScD and leverages the MANTID framework. ADARA is expected to be deployed across SNS beam lines by Fiscal Year (FY) 2015. The third foundational project is the development of the next generation SNS instrument control system that addresses reliability and flexibility of beam lines by leveraging a common control framework that is widely used at other facilities. This FY 2014-2016 effort will incorporate developments in ADARA and MANTID to allow intelligent feedback to the instrument control system, optimizing use of neutron beam time.

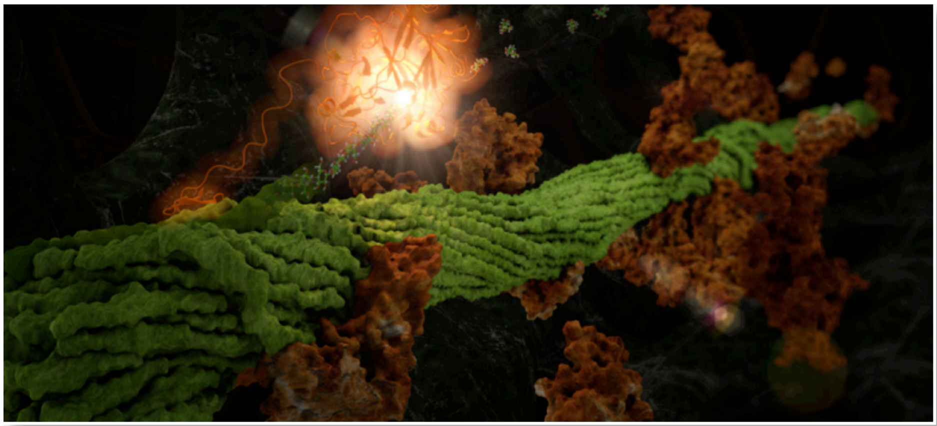


Figure 22. Cray XT5 simulation model of lignocellulosic biomass (lignin and cellulose) together with an artist's impression of a cellulase enzyme hydrolyzing the cellulose for subsequent conversion to biofuel. Neutron scattering in combination with computer modeling is playing an important role in understanding biomass structure and its conversion to biofuels. Our vision is to integrate neutron scattering with high performance computing across all five science priority areas.

The next level of targeted development addresses the ways researchers address scientific questions that require a combination of research tools and skill sets. The Scientific User Facilities Division of BES is supporting a two year pilot project with the Advanced Photon Source (APS) to develop the cataloging, data transfer and management, and co-refinement software for experimental neutron and X-ray diffuse scattering data. This will enable advances in understanding materials using multiple probes and extend to other science areas and instruments beyond this pilot.

Integration of Neutron Scattering with High Performance Computing

Our data and modeling vision is to tightly integrate neutron scattering with ORNL strengths in high performance computing and materials theory. A recent workshop, Data and Communications in Basic Energy Sciences: Creating a Pathway for Scientific Discovery, brought together leading researchers from BES facilities and DOE Office of Advanced Scientific Computing Research (ASCR). Three needs were identified: (1) integrating theory and analysis into the experimental workflow, (2) moving analysis closer to experiment, and (3) matching data management access and capabilities with advancements in detectors and sources. Funding was allocated through BES to establish CAMM, with the aim to integrate the techniques of high performance computational simulation and modeling with the analysis of neutron scattering data. The scientific impact of such integration is twofold. First it allows the power of computational modeling to provide predictive guidance in the interpretation of the experimental data. Second, by refining the computational predictions against the experimental data, it improves the computational model so that its predictions are more reliable and accurate. This integration will be particularly important in the emerging areas of multiscale complexity and interfaces in our science priorities.

Sources

SNS Accelerator and FTS Target Upgrades

Increasing SNS accelerator beam power provides a direct increase in neutron flux intensity at all beam lines. SNS accelerator and FTS target systems are designed to operate at 1.4 MW, and this capability will be demonstrated in the 2013-2014 period with limited high-power operation aimed at identifying areas that require improvements to ensure reliability. By 2016, SNS staff intend to operate at its design power of 1.4 MW with a goal of 90 percent availability. Beam power will be increased from the present ~1 MW level through a combination of increases in beam energy, beam current and pulse length.

Ensuring reliable source operation is critical to providing effective support for neutron scattering science. Major concerns are adequate target lifetime at higher power operation, accelerator equipment reliability at the higher duty factor and power levels, and equipment obsolescence issues. New target designs currently being developed will facilitate post-irradiation inspections to better understand damage and failure mechanisms. Cavitation-induced erosion of the vessel wall remains an operating concern. Gas bubble injection is proposed as a mitigating mechanism, and development efforts are in progress.

The inner reflector plug (IRP) assembly in the target moderator system will reach its end of life in 2016, and will be replaced by an IRP of similar design at this time. During this replacement the IRP coolant will be transitioned from H_2O to D_2O, which will provide a 15-20 percent improvement in neutron flux. Even further improvement in the coupled reflector and moderator assembly is possible with appropriate system

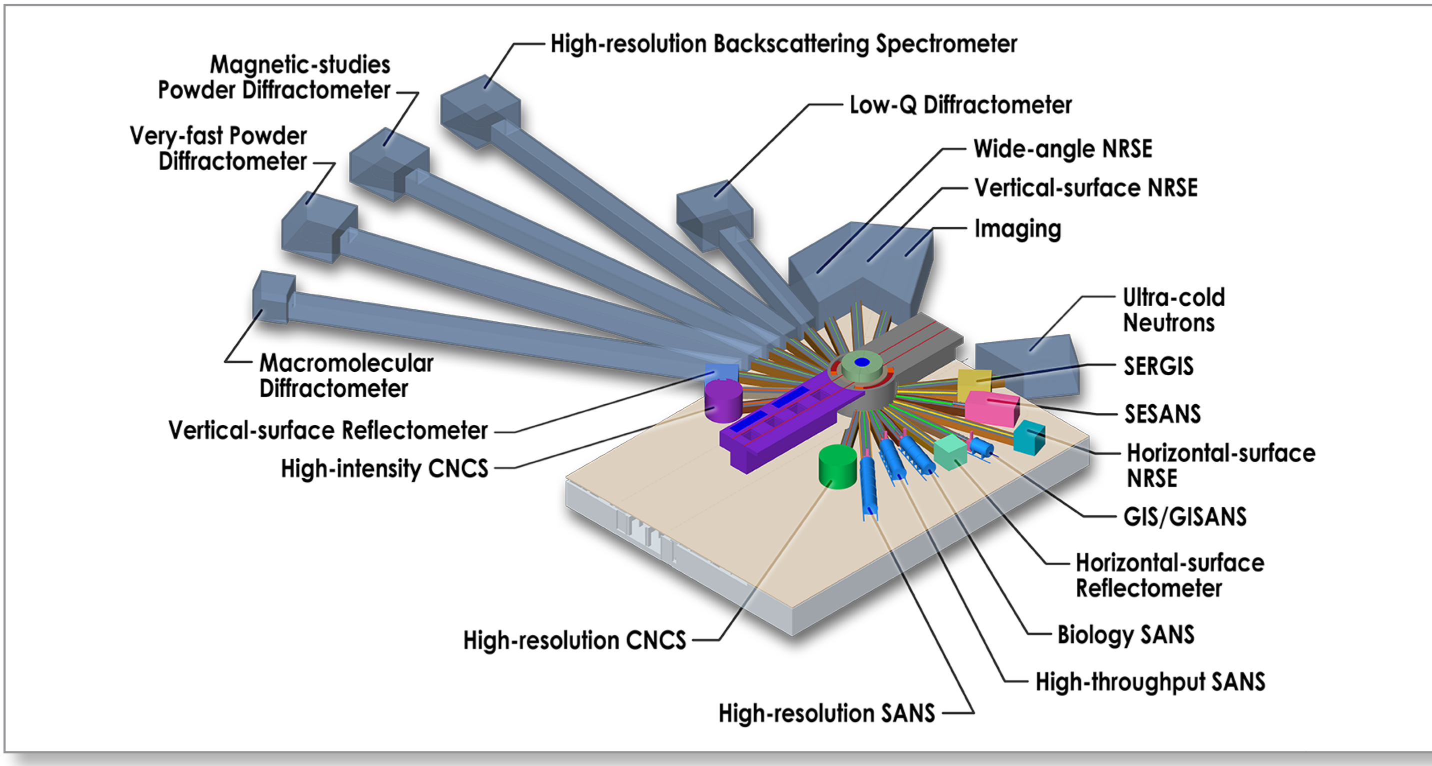


Figure 23. A reference suite of instruments and neutron beam layout for the STS.

optimization. A redesigned IRP/moderator system offering up to 50-70 percent improvements in the neutron fluxes from some moderators is planned for installation in the following IRP change-out, occurring in 2021.

Increasing superconducting cavity gradient levels using a novel in-situ plasma processing technique, currently being developed, will increase the accelerator beam energy to the design level of 1 GeV. Also, as the pulse length is increased to the full 1 ms, equipment will be further stressed, and efforts to mitigate reliability concerns are being deployed. For example, improvements are underway in cooling and pulse shape modulation for the high power pulsed electrical equipment. For the ion source, an approach that removes the radio frequency antenna from the harsh plasma environment is being developed. Some components are no longer available for the custom electronics systems used in accelerator radio frequency control, beam instrumentation, and timing systems. These systems need to be updated with a sustainable parts supply, and replacement of these systems is expected to take about five years.

Second Target Station

SNS was designed from the outset to accommodate a STS, effectively doubling the neutron science capacity of the accelerator infrastructure, and adding significant science capabilities to the ORNL neutron scattering instrument suite (Figure 24). The first step in the STS project preparation is finalizing the requirements for the source characteristics, required proton beam parameters and the initial instruments. Decisions on the source pulse frequency, power level and the instrument layouts will provide the basis for proceeding with the planning

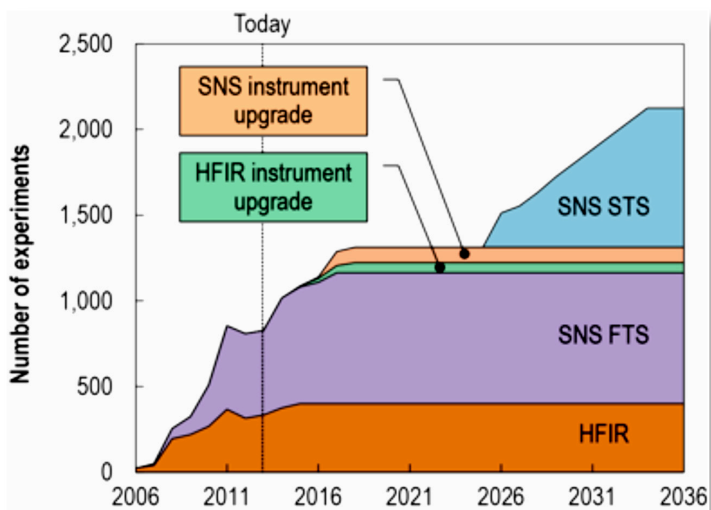


Figure 24. Neutron scattering experiments at HFIR and SNS. The STS projection assumes a nearly constant ramp to 20 instruments.

activities needed for CD-1. These decisions will be aided by a series of focused workshops involving the neutron scattering community in 2014. Finalized source requirements and instrument footprints will be followed with the development of a Technical Design Report (TDR) which will provide a basis for the CD-1 completion by the end of 2015. This scenario assumes some development resources available in 2014 for the initial TDR preparation. Detailed cost estimates will be prepared in 2016-2017, aiming at a CD-2 completion in mid-2018. Construction for this project is expected to cover a six year period, ending in 2024.

A key element in the STS plan is increasing the beam power. This increase is critical to enable delivery of the required beam intensity to the STS, as well as to increase the beam power delivered to the FTS to about 2 MW. The accelerator upgrades will roughly double the beam power for a fraction of the cost of the original accelerator, providing a cost-effective increase of the neutron intensity in all the beam lines. A key driver is the expected need to deliver 400-500 kW beam power at 10 Hz to the STS. To accomplish this the proton beam energy will increase by 30 percent and the beam current will increase ~50 percent to 50 mA. This power increase was anticipated during the original construction, and additional room is available in the linac tunnel and linac support building for nine additional superconducting radio frequency cryo-modules, adequate to provide the 30 percent energy increase. Almost all of the transport line and ring magnets were built to handle the 30 percent higher beam energy. The increased beam current will require some ion source development and improved radio frequency high voltage power supply capability to support the increased beam loading. Targets capable of handling the higher power also need to be developed, leveraging the lessons learned in 1-1.4 MW operation.

Beyond the equipment implementations needed to double the beam power, there are other areas of research and development needed to assure reliable operation at and above 2 MW. Beam instability becomes a major concern at the higher required stored beam intensities, and damping systems to counter these instabilities need to be developed. Survival of stripper foils at the much higher beam powers is a potential issue, and development of long lead-time alternatives such as laser stripping are being pursued. Finally, the issue of beam loss and equipment activation becomes even more critical at higher operational power. SNS already has world-class low fractional beam loss for a high power proton accelerator, but further improvements are necessary to maintain the same level of equipment activation as higher operational powers are adopted. Development of beam instrumentation capable of measurements with dynamic ranges of ~ 10^5 are needed to better understand and control the “halo” edge of the beam, which is a major contributor to beam loss.

Neutronics – Source Optimization

Optimization of neutron source characteristics can result in significant gains (factors of 2 to 10 relative to the present day FTS moderator performance) in ultimate instrument performance. Improving existing sources requires early investment in component development as conceptual design and optimization efforts typically require several years or more, followed by detailed engineering and procurement.

Optimizing the moderator performance at SNS-FTS and STS requires understanding and control of the ortho/para ratio of the moderators. Gains of 40-60 percent can be realized for the coupled moderators on FTS by optimizing the volume of a pure para-hydrogen moderator. Development of in situ methods for determining the ratio under operating conditions and development and design of a catalyst system are fundamental to achieving these gains for FTS. This technology is critical to achieving the brightest moderators on STS. Advanced moderator concepts employing more exotic materials such as ^{15}N ammonia, pelletized-solids, or nano-particle reflectors hold the promise for the highest performance gains but require years of development to reach the robust level of performance required for an operating user facility. ORNL is part of an international collaboration in this area and conducts an experimental program in collaboration with researchers at the Indiana University Low Energy Neutron Source (LENS) facility.

Extending the life of SNS target will improve operational reliability while reducing costs. ORNL will collaborate with the Japan Spallation Neutron Source (JSNS) at J-PARC on gas injection technologies for mitigation of cavitation induced erosion while continuing its post-irradiation target inspection program to better understand end-of-lifetime parameters such as radiation damage to the steel vessel.

EXECUTING THE PLAN

Executing the plan

Execution of this strategic plan will be accomplished through a series of concurrent activities that include: continued community engagement; further integration with ORNL science and technology organizations and capabilities; increased production from the two neutron sources; optimization of the current suite of instruments; execution of an additional instrument upgrade project (SING III); and continuation of the STS Project. Beam line and source co-optimization are staged to minimize disruption to ongoing user operations.

Community Engagement

This plan continues our commitment to building and supporting a broad user community that addresses fundamental and discovery-based questions in disciplines including physics, chemistry, geology, biology and medicine, and materials and engineering science. One of the most important parts of the planning process is an ongoing consultation with the scientific research community to continually refine the science priorities. This will include a series of focused scientific and technical workshops organized by our staff. Guided by the workshop reports, ORNL will make a final decision on prioritization of instruments, source and enabling technologies.

Integration with ORNL

A guiding vision arising from all of the science priority areas is to tightly integrate neutron scattering with other strengths of ORNL such as high performance computing and materials synthesis. Integrating neutrons with high performance computing will be achieved in part by executing the CAMM. It will also be achieved by creating strategic positions in ORNL's CCSD that will guide the development of scalable applications for neutron science, and act as science liaisons to OLCF. Integrating neutrons with chemical and biological materials synthesis will be achieved through partnerships with expertise and resources in the Physical Science Directorate and the Energy and Environmental Sciences Directorate.

Increased Production from SNS and HFIR

To meet the increasing demand for neutron scattering capacity, two actions are planned to increase capacity. First, it is planned that HFIR and SNS will both achieve optimal operating schedules that maximize available neutron production hours. Currently, HFIR and SNS neutron production has been limited because of budgetary constraints. Restoration of operational funds to the facilities would enable HFIR to restore two operating cycles and SNS to increase its neutron production scheduled hours to 5,000 annually. Second, funding will enable construction of instruments on the undeveloped beam lines at SNS (4 beam lines) and HFIR (2 beam lines).

Optimization of the Current Suite of Instruments

The remaining beam lines being built as part of SING Programs (I and II) will be completed, commissioned, and brought into the user program by 2016. Scientific productivity and priority reviews will be conducted for operating instruments on regular schedules. Decisions on the continuation, upgrade, or scope change for operating instruments will be based on the recommendation of the reviews.

Advancement of Enabling Technologies

Continued improvement in detector performance, neutron optics sample environment, laboratory capabilities and data analysis will provide the technical foundations enabling the beam lines to meet user expectations and scientific objectives. Advances will be achieved through targeted use of operations funds focused on achieving specific outcomes and via external industry and university collaborations that leverage DOE investments in the SBIR/STTR program and other agency funding opportunities. We will continue to forge collaborations with leading national and international neutron facilities in areas of common interest.

SING III Project

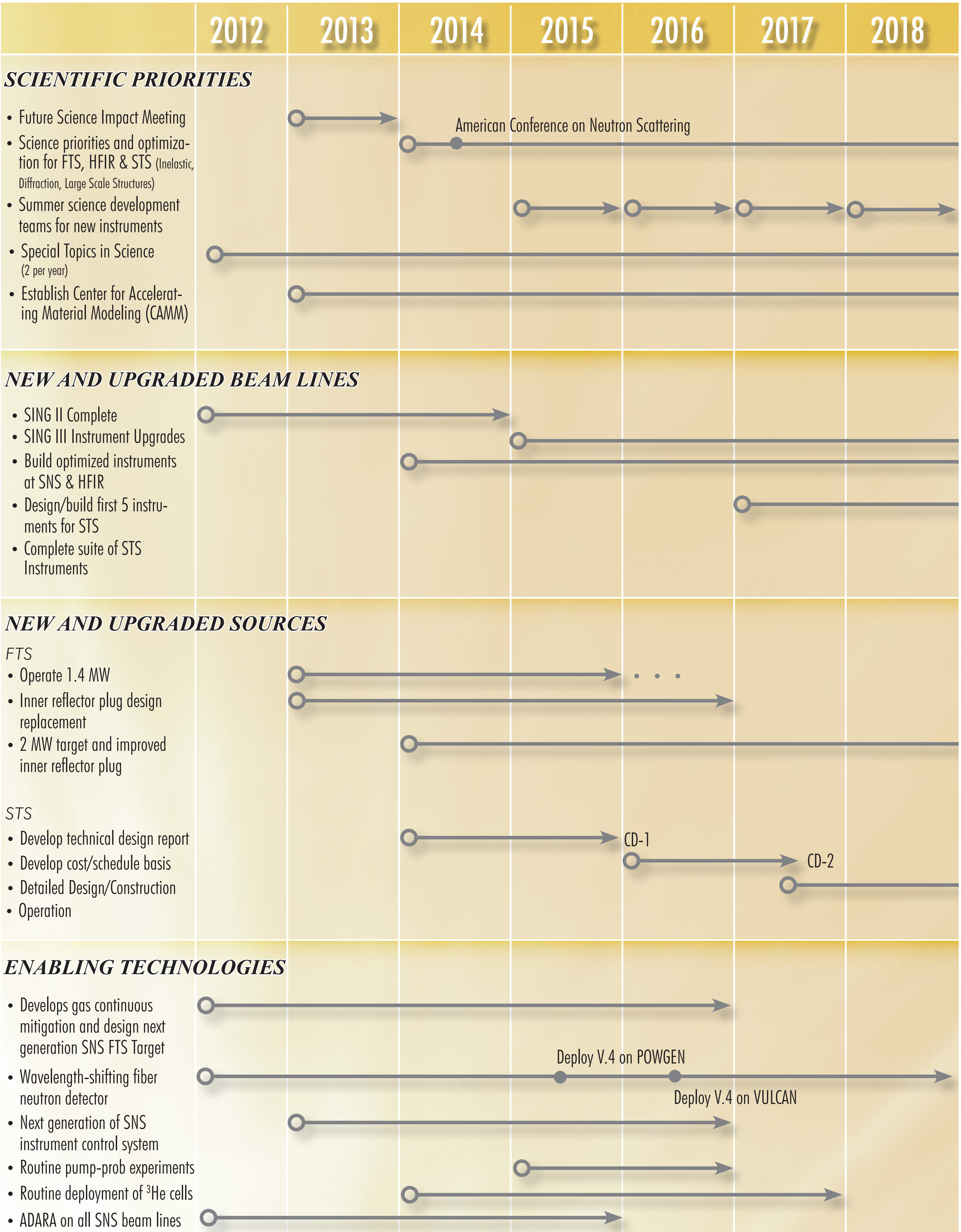
A new BES SING III project is planned to enhance existing beam line capabilities in line with their original design performance and user expectations over the period from 2015-2019. This beam line upgrade plan includes upgrading detectors, neutron optics, sample environments, and developing new data analysis and visualization techniques.

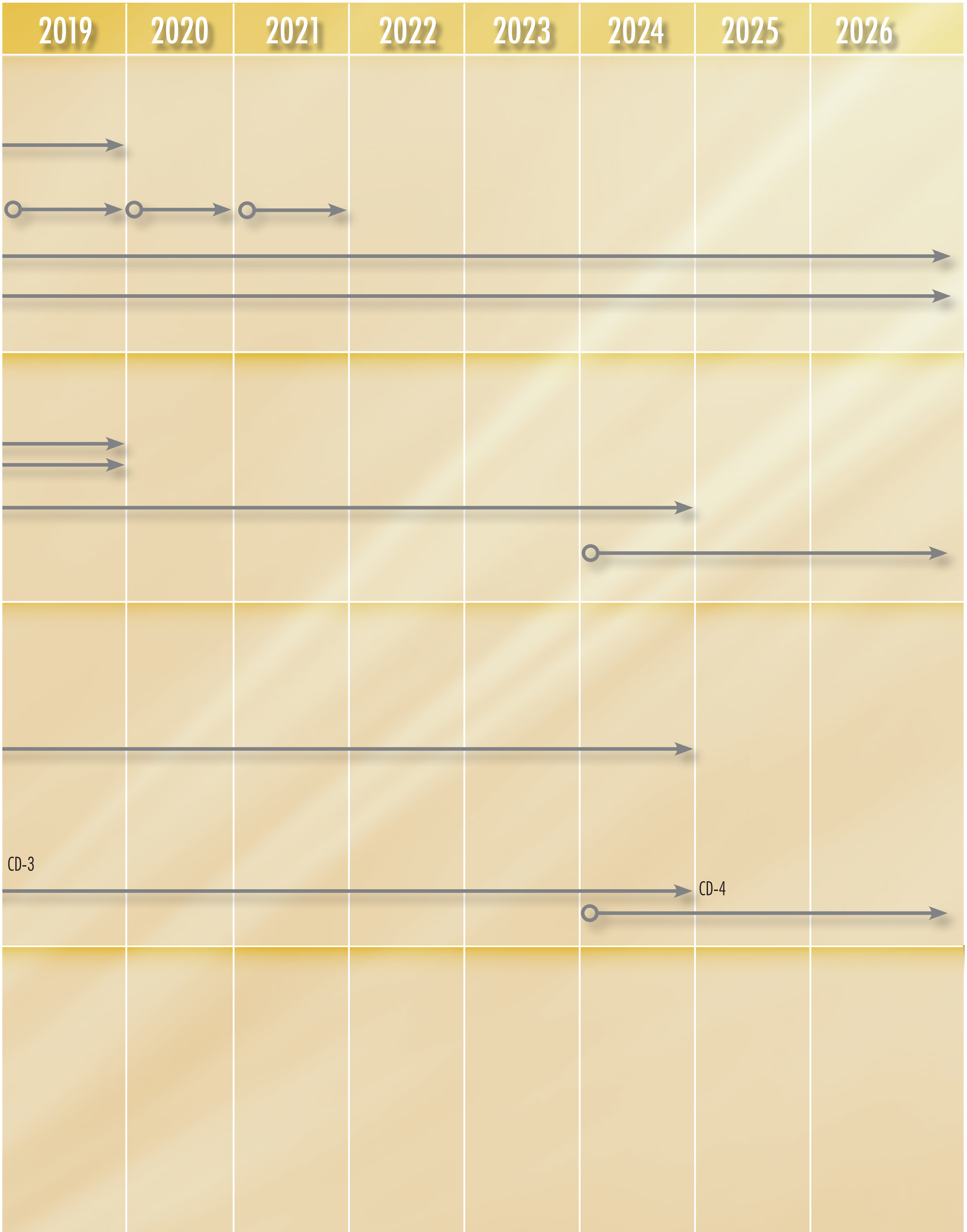
Second Target Station (STS)

ORNL will complete the first set of beam lines on the STS in fall 2024. All beam lines will be evaluated and optimized based on the source capabilities of HFIR, FTS, and STS. This process will identify areas in which new scientific and technical expertise is needed; therefore, it is anticipated that target hires will be needed to bring certain expertise in-house. In some technological areas leadership expertise exists at other facilities or institutes, and appropriate partnerships will be established to accelerate development.

Execution of this comprehensive plan will place the United States in a forefront position in international neutron science for at least the next two decades. Failure to act will have a significant negative impact on the United States' ability to remain competitive in solving the grand scientific challenges that support energy research and development.

STRATEGIC TIMELINE


2012
2013
2014
2015
2016
2017
2018
SCIENTIFIC PRIORITIES
• Future Science Impact Meeting
• Science priorities and optimization for FTS, HFIR & STS (Inelastic, Diffraction, Large Scale Structures)
American Conference on Neutron Scattering
• Summer science development teams for new instruments
• Special Topics in Science (2 per year)
• Establish Center for Accelerating Material Modeling (CAMM)
NEW AND UPGRADED BEAM LINES
• SING II Complete
• SING III Instrument Upgrades
• Build optimized instruments at SNS & HFIR
• Design/build first 5 instruments for STS
• Complete suite of STS Instruments
NEW AND UPGRADED SOURCES
FTS
• Operate 1.4 MW
• Inner reflector plug design replacement
• 2 MW target and improved inner reflector plug
STS
• Develop technical design report
CD-1
• Develop cost/schedule basis
CD-2
• Detailed Design/Construction
• Operation
ENABLING TECHNOLOGIES
• Develops gas continuous mitigation and design next generation SNS FTS Target
• Wavelength-shifting fiber neutron detector
Deploy V.4 on POWGEN
Deploy V.4 on VULCAN
• Next generation of SNS instrument control system
• Routine pump-prob experiments
• Routine deployment of ^{3}He cells
• ADARA on all SNS beam lines


2019
2020
2021
2022
2023
2024
2025
2026
CD-3
CD-4

APPENDIXES AND ACRONYMS

Appendix A: Optimizing Instruments and Techniques Across ORNL Neutron Sources

Performance of ORNL Neutron Sources

The two existing forefront neutron facilities, SNS-FTS and HFIR, combined with the proposed long-wavelength SNS-STS will support the most potent and complete range of neutron beam facilities available anywhere in the world, now and in the foreseeable future. As shown in Figure 1, the 60 Hz SNS-FTS water moderator provides the greatest time-averaged brightness among existing pulsed sources in the wavelength range of particular importance for powder diffraction at small d-spacings (high momentum transfers) and high energy transfer inelastic spectrometers. The accelerator power upgrade that is part of the STS Project will increase FTS performance by 40 percent (dashed line). At 5 MW, the ESS is anticipated to produce a higher time-averaged brightness even for its cold moderator in this wavelength range, but the peak brightness of a 2 MW FTS will be higher as shown in Figure 2. HFIR cold source is comparable to the world's best reactor cold sources and provides the highest time-averaged flux of cold neutrons of the ORNL sources, approximately x10 that of a STS. In the thermal range, HFIR provides the highest time-averaged flux of the ORNL sources at about x40 that of FTS. As envisioned, a 10 Hz STS optimized for the production of long-wavelength neutrons will provide the highest peak brightness of any neutron source in the world, existing or planned (Figures 1 and 2). Reducing the STS moderator dimensions to 5 x 5 cm^2 will improve the brightness an additional factor of 1.7 relative to the 10 x 10 cm^2 moderator shown in Figure 1.

The three ORNL facilities provide a unique opportunity to match neutron scattering techniques and instrument design to the source characteristics that deliver the best performance. ORNL will be the only laboratory in the world to provide neutron scattering capabilities optimized across such a diverse set of sources.

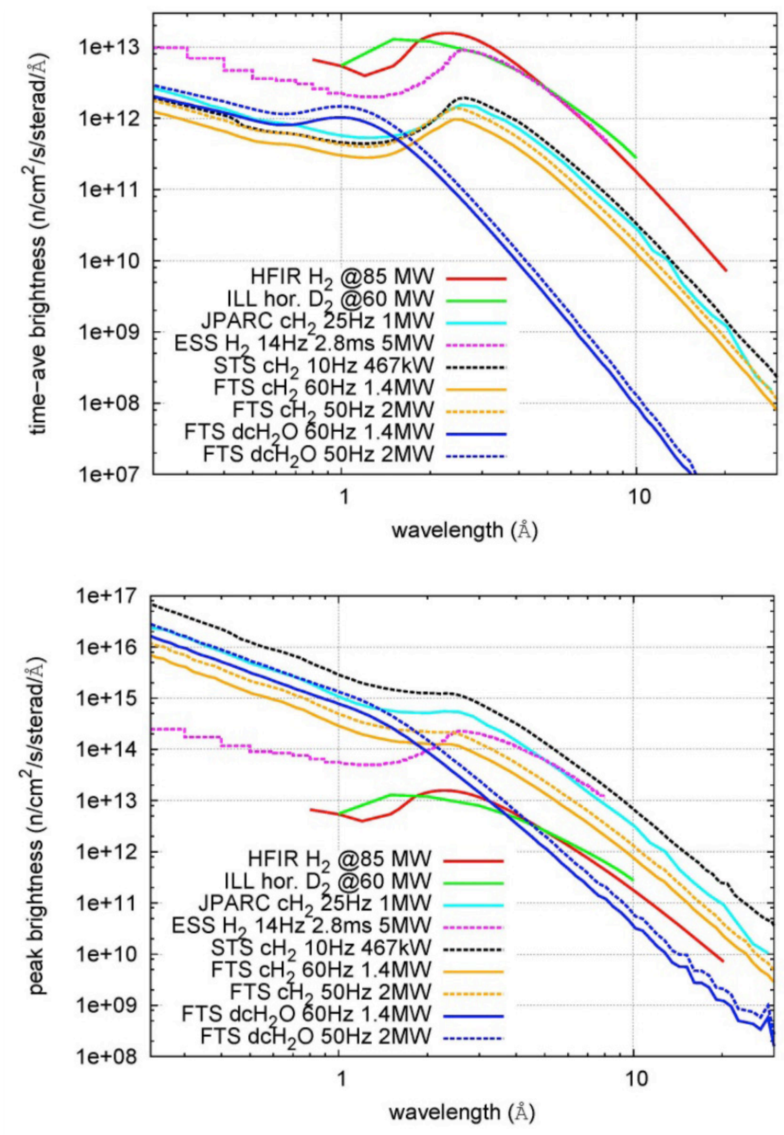


Figure 1. Moderator and cold source performance from leading and proposed reactor and pulsed spallation neutron sources. Solid curves represent the full baseline performance of existing sources while dotted-dashed curves represent future facility plans. The upper plot (a) shows the time averaged brightness of the moderators and cold sources while the lower plot (b) shows the peak brightness. The performance of some neutron scattering instruments scales with the average flux as in (a), while for others, performance scales with the maximum number of neutrons that can be generated in a short period of time as in (b). The performance of remaining instruments scales somewhere between these two extremes. This figure also appears on page 12 of this plan.

B. Instrument Optimization

The operating frequency, ν (Hz), of a pulsed spallation source is a key parameter in optimizing its neutron scattering instruments. The neutron wavelength bandwidth, Δλ (Å), available to the instrument is inversely proportional to ν and the length, d (m), of the instrument, $\Delta\lambda=3956/((d\cdot\nu))$. Higher source operating frequencies favor shorter instruments or instruments that use a small Δλ. For elastic techniques, the gains in employing TOF techniques are proportional to the number of useful instrument resolution elements available within this wavelength band. For inelastic instruments, gains are proportional to the peak neutron intensity at the desired λ and the ratio of the source frequency to the optimum instrument operating frequency. Repetition rate multiplication schemes can address the latter.

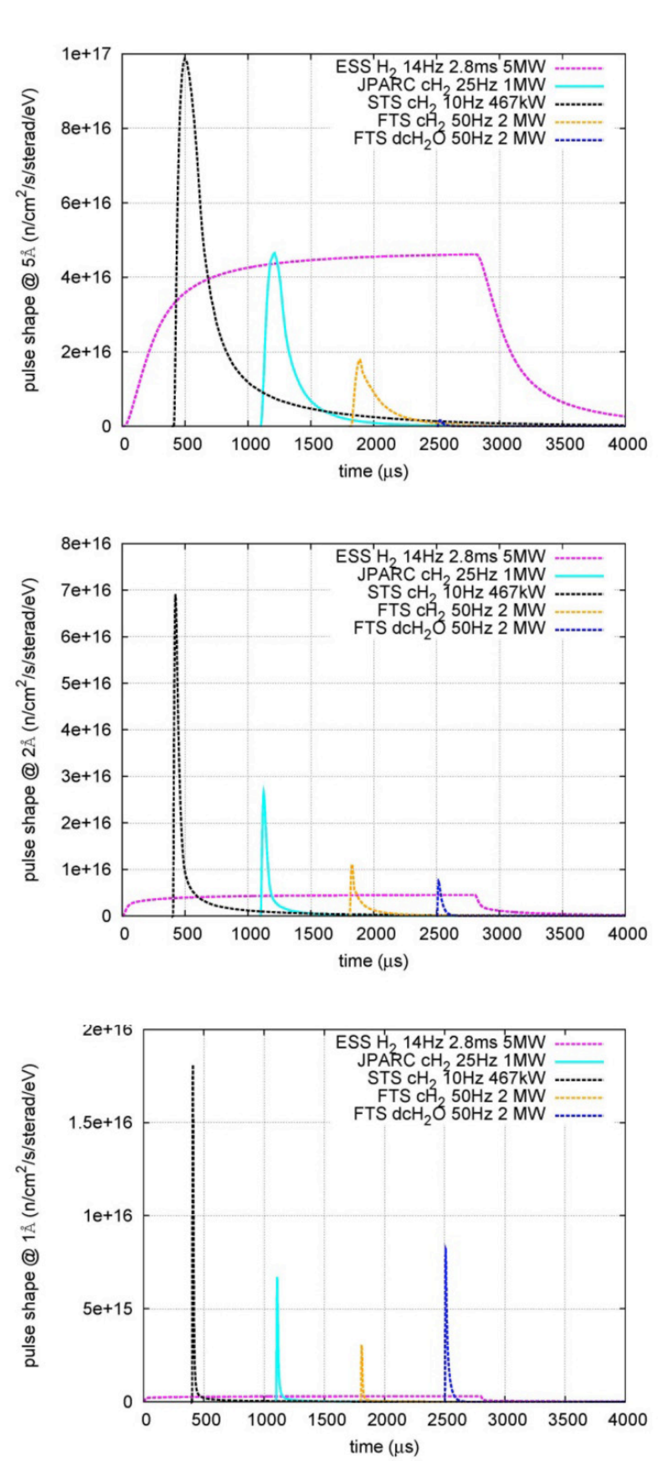


Figure 2. Moderator time distributions for pulsed spallation neutron sources: λ = 5 Å (a), λ = 2 Å (b), λ = 1 Å (c).

Neutron scattering techniques and instruments that are optimized to use a small number of resolution elements are best optimized to a reactor based, continuous source that produces the greatest neutron time-averaged flux at the desired λ.

Figure 3 is an optimal performance map of elastic scattering techniques across ORNL neutron sources. The performance of most elastic scattering instruments depends on its range of accessible momentum transfers, Q, its Q-resolution, and its effective count rate. On most elastic instruments the Q-resolution is proportional to the wavelength resolution because the instrument geometry is designed to match geometrical contributions to the wavelength term. The x-axis in Figure 3 is the desired wavelength resolution expressed as δλ/λ. The y-axis is the number of these wavelength resolution elements required for any given measurement. For example, a powder diffractometer with a δλ/λ of 0.0005 will use about 4600

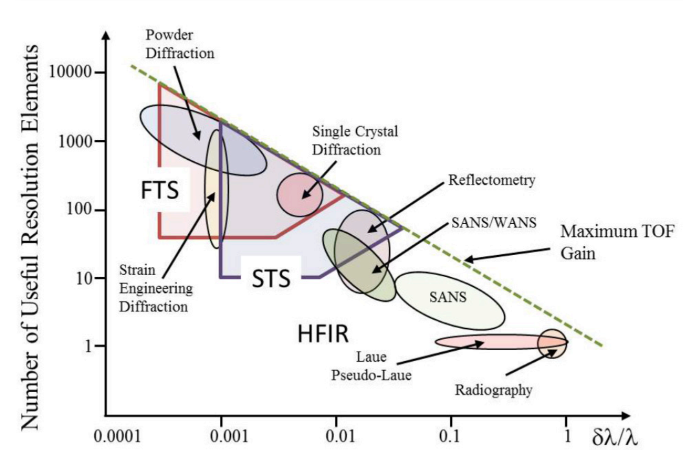


Figure 3. Optimal performance map of elastic scattering instruments across the ORNL neutron sources. Within the labeled boxes, the performance of the ORNL pulsed sources are expected to exceed that of HFIR. Outside the boxes, HFIR will obtain a desired data set more quickly.

resolution elements across a wavelength band from 0.5 to 5.0 Å. The approximate regimes of various elastic scattering techniques are indicated by the ovals. The maximum possible gain due to time-of-flight techniques is proportional to (δλ/λ)-1 and is indicated by the dashed line. The figure compares the performance of the two pulsed sources scaled to HFIR. Within the labeled boxes, we expect the pulsed source performance to exceed that of HFIR; outside the boxes, HFIR will obtain a desired set of data more quickly. Notice that this simplified graph ignores features such as background which can determine outcomes in some cases. The lower boundaries between HFIR and the pulsed sources are determined by the ratio of the time-averaged neutron flux of SNS moderators and HFIR. The potential gain provided by the pulsed sources relative to HFIR increases as one moves upward in the chart. For example, at a δλ/λ of 1 percent, the STS can potentially measure a given sample as quickly as HFIR provided more than 10 resolution elements are required. If 100 resolution elements are required, the STS could potentially make a measurement 10 times faster than HFIR. While there is a region in which FTS and the STS overlap, there are also regions where each excels. The same conclusion applies to a comparison of HFIR with either pulsed source.

Figure 4 maps the performance of inelastic neutron scattering instruments. With the exception of backscattering and neutron spin echo, most inelastic studies use an energy resolution of a few percent and differ mainly in the magnitude of the incident energy. To separate the instruments we choose the x-axis as the energy resolution (δE) in meV and the y-axis as the

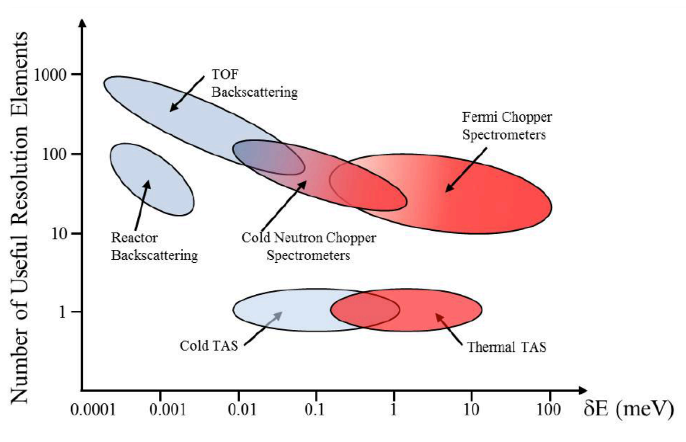


Figure 4. Performance map of the inelastic spectrometers. The colors indicate the incident neutron energy with red signifying thermal to epi-thermal neutrons and blue, cold neutrons.

number of energy resolution elements required for the experiment. Instruments to the right of this chart tend to use thermal to epi-thermal neutron energies, while those to the left tend towards use of cold neutrons, as indicated by the red and blue shading. The relative performance of the sources depends on the ratio of the time-averaged neutron flux modified by the number of resolution elements required. FTS produces 40x less thermal neutrons than HFIR, so only in cases where more than 40 resolution elements are required could FTS obtain data of a given quality more quickly than HFIR. As the plot indicates, Fermi chopper instruments fall into this category, but they are not competitive with triple-axis spectrometers (TAS) at HFIR when only a few resolution elements are required. Thus, TAS will always perform best at HFIR. The performance of TOF chopper spectrometers scales with the peak neutron flux at the desired wavelength, provided the source is operated at a frequency that gives the desired number of resolution elements. The Fermi chopper spectrometers are best matched to the performance of the FTS water moderator. For cold neutron chopper spectrometers, the STS coupled H_2 moderator has about 5 times the peak brightness of the FTS moderator (see Figure 2). Assuming repetition rate multiplication is equally effective at both sources, these instruments will be best sited at the STS. TOF backscattering spectrometers excel in their ability to sample a large dynamic range of energy transfers. The highest energy resolution requires the use of long wavelength neutrons (≈20 Å) and long beam lines, favoring STS. At shorter wavelengths, reasonable dynamic ranges can be obtained at the higher operating frequency of FTS and its poisoned, decoupled moderators provide ideal pulse widths. As was the case for the elastic scattering instruments, HFIR tends to be best matched to techniques which employ the smallest number of resolution elements. There is a significant overlap in capabilities between FTS and STS to support cold neutron TOF spectroscopy and highly effective cold neutron chopper and backscattering spectrometers can be built at each source.

Appendix B: Planned Beam Line Upgrades

CORELLI (BL-9): Designed for studies of single crystal elastic-only diffuse scattering as part of SING II, CORELLI will initially have about 1/3 of its detector coverage upon completion in 2014. Filling out the detector coverage is imperative to maximize the Q-range and data rate.

POWGEN (BL-11A): We will improve the signal to noise on POWGEN by a factor of 5 by expanding the detector coverage and adding argon-filled secondary collimation.

Bio-SANS (CG-3): Our strategy for small angle scattering beam line Bio-SANS is to extend its q-range and to develop new sample environments that will enable multi-length scale time-resolved studies that characterize dynamic functional assemblies, disorder and flexibility, and biological membranes in complex biological systems. A creative multi-bank detector concept is proposed that will provide uniquely broad simultaneous q-range coverage compared to other SANS beam-lines in the world, with an unprecedented dynamic range (qmax/qmin) exceeding 250 compared to the currently available range of 20.

MaNDi (BL-11B): The detector coverage of crystallographic beam line will be enhanced by the addition of up to 20 additional detectors that will nearly double its capability, allowing for the study of smaller samples and more complex systems such as membrane proteins.

IMAGINE (CG-4D): The crystallography beam line IMAGINE will be equipped with a diverse variety of sample environment equipment including cryogenic temperatures, high temperature, and high pressure. These capabilities will extend the scientific reach of IMAGINE beyond biology to energy and quantum materials.

Fixed-Incident Energy Triple-Axis Spectrometer (HB-1A): Exotic states of matter in systems such as itinerant magnets, thin films, and extended electron systems, often result in weak magnetic moments and can only be effectively studied with sufficient background reduction as is achieved on the HB-1A fixed energy triple-axis spectrometer. To fully optimize for such measurements, it will be essential to maximize the accessible Q-range which will be enabled by developing a novel, lifting counter diffractometer with energy discrimination for HB-1A to facilitate out-of-plane Q coverage.

WAND (HB-2C): Rapidly mapping out volumes of reciprocal space in single crystal samples in the presence of a variety of sample environment equipment is crucial to understand the complex phase diagrams in materials such as frustrated magnets and materials related to high-Tc superconductors. Modernizing the US-Japan WAND instrument will allow for such measurements with a new sample table, detector shield, and a large 2d position sensitive detector.

Neutron Powder Diffractometer (HB-2A) and Four-Circle Diffractometer (HB-3A): For single crystal studies, we will expand the capabilities of the HB-3A diffractometer by the inclusion of a 2d detector, expanded low temperature and magnetic field capability, and a polarized beam option for separation of nuclear and magnetic scattering. For powder studies, the HB-2A powder diffractometer will be modernized by the inclusion of a large 2D PSD and an oscillating radial collimator to dramatically improve the data collection rate facilitating measurements with smaller samples and faster parametric studies.

SEQUOIA (BL-17): Measurements of the excitations in low dimensional materials such as high-TC superconductors are enhanced by symmetric in-plane and out-of-plane detector coverage. The SEQUOIA detector coverage will be expanded to full capacity to enable symmetric Q coverage at low Q, improving efficiency for such studies.

Polarized Triple-Axis Spectrometer (HB-1) and Triple-Axis Spectrometer (HB-3): To improve this complementarity, we will modernize the HB-1 and HB-3 triple-axis spectrometers by upgrading the sample table and analyzer/detector enclosure allowing for introduction of a double focusing analyzer resulting in significant improvements in signal to background and expanded ability to utilize complex sample environments.

CNCS (BL-5): To facilitate such measurements, the signal to noise of CNCS will be improved by an order of magnitude by doubling the detector coverage, reconfiguring the chopper system to allow simultaneous measurements with multiple energies, and adding a T0 chopper for background suppression.

Cold Neutron Triple-Axis Spectrometer (CG-4C): Novel properties often emerge from quantum magnets with competing interactions which often possess small energy scales, well matched to cold neutron inelastic instruments like CNCS and the US-Japan instrument CTAX. To optimize CTAX for parametric studies, to complement the mapping capability of CNCS, we will incorporate a new, double focusing analyzer and replace the bender on the CG-4 guide which will improve the signal for many problems of interest by a factor of 5.

EQ-SANS (BL-6): An improved large sample area on EQ-SANS will create easy access for operation of large exotic environments (e.g. coquette-geometry rheometers) while the addition of wing detectors will provide a large dynamic Q-range for kinetic and pump-probe experiments to take full advantage of the intensity and high resolution.

GP-SANS (CG-2): A set of fixed, staggered set of planar detector banks plus a high resolution beam-stop detector will permit coverage of a wide Q range without moving the detector. This will enable new studies in kinetics of colloids, polymers, and surfactants to permit parametric studies of meso-scale structures.

Liquids Reflectometer (BL-4B) and Magnetism Reflectometer (BL-4A): Improvements planned for the both the Liquids and Magnetism Reflectometers will provide new capabilities to perform off-specular scattering to resolve in-plane structures in thin films with features from 10nm—20 µm. In addition, new detectors will permit both instruments to measure reflectivity over larger dynamic ranges with shorter data transfer rates.

BASIS (BL-2): Investigation of weakly scattering systems such as Li-ions and more accurate determination of the geometry of localized diffusive motions with high energy resolution will be enabled on BASIS. The addition of new analyzer panels will improve the signal-to-noise ratio, produce 50 percent faster measurements, and broaden the Q-range at energy resolution of 11 µeV.

NSE (BL-15): Parametric studies of the dynamics of complex fluids in solution are needed to enhance our knowledge of polyelectrolyte interactions. Improved polarizing optics for increased flux, improved data reduction to optimize data quality, and the addition of improved correction coils will improve the data collection times and increase the Fourier time scales on NSE.

TOPAZ (BL-12): High resolution single crystal neutron diffraction provides unique, structural information for a diverse set of materials including metal hydrides, perovskites, organometallic complexes and studies of hydrogen bonding. TOPAZ will be the general purpose single crystal diffractometer for chemical crystallography at SNS. To enhance the capabilities of this instrument, 12 new detectors will be added to give up to 50 percent higher count rates and more complete crystallographic coverage for individual samples. Workhorse low-temperature sample environments will be developed.

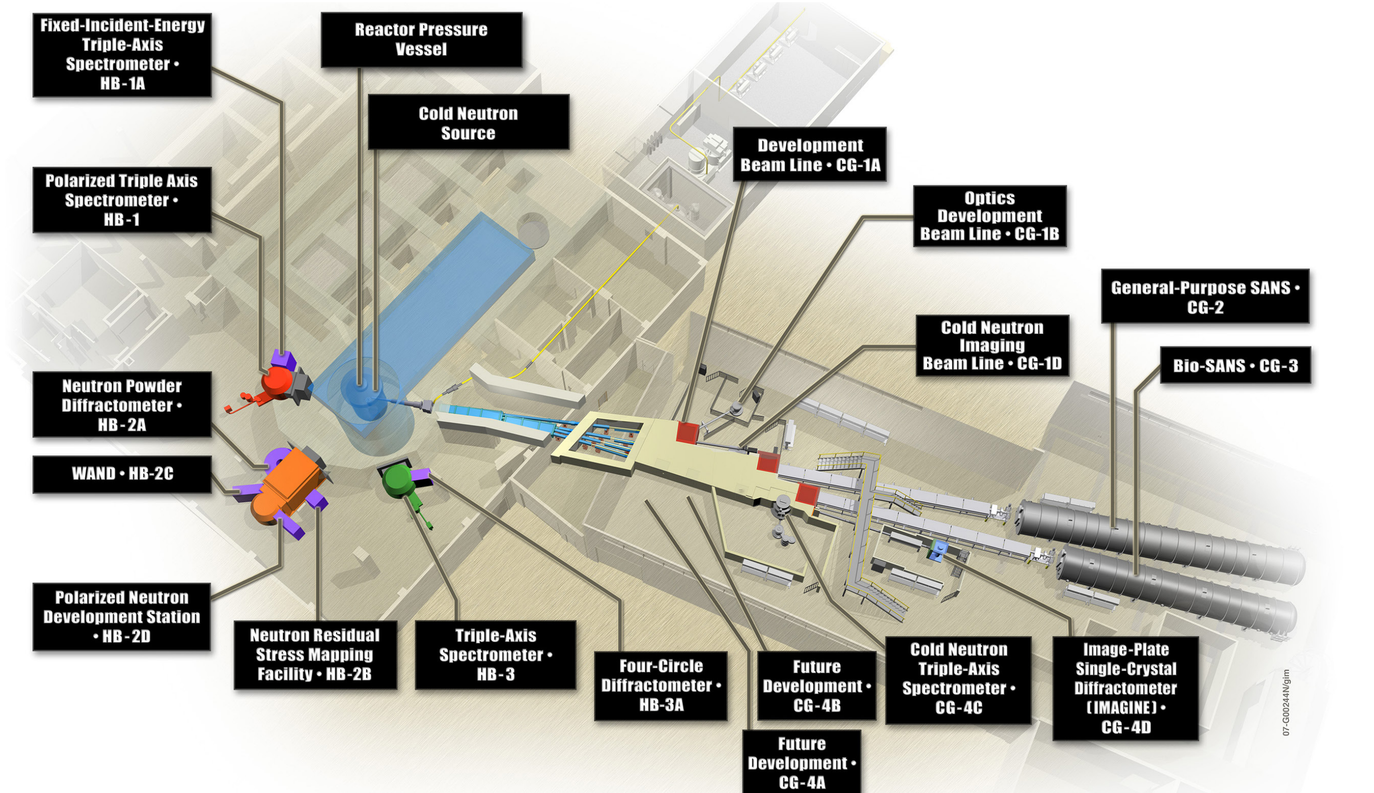
NOMAD (BL-1B): Expansion from the current detector coverage of 4 steradians to the originally planned detector coverage of 8.2 will enable NOMAD to routinely perform such measurements with high statistical precision on small and/or weakly-scattering samples.

SNAP (BL-3): Upgrading the Anger camera detectors on SNAP, as has been successfully demonstrated on TOPAZ, will enable single crystal, high pressure diffraction.

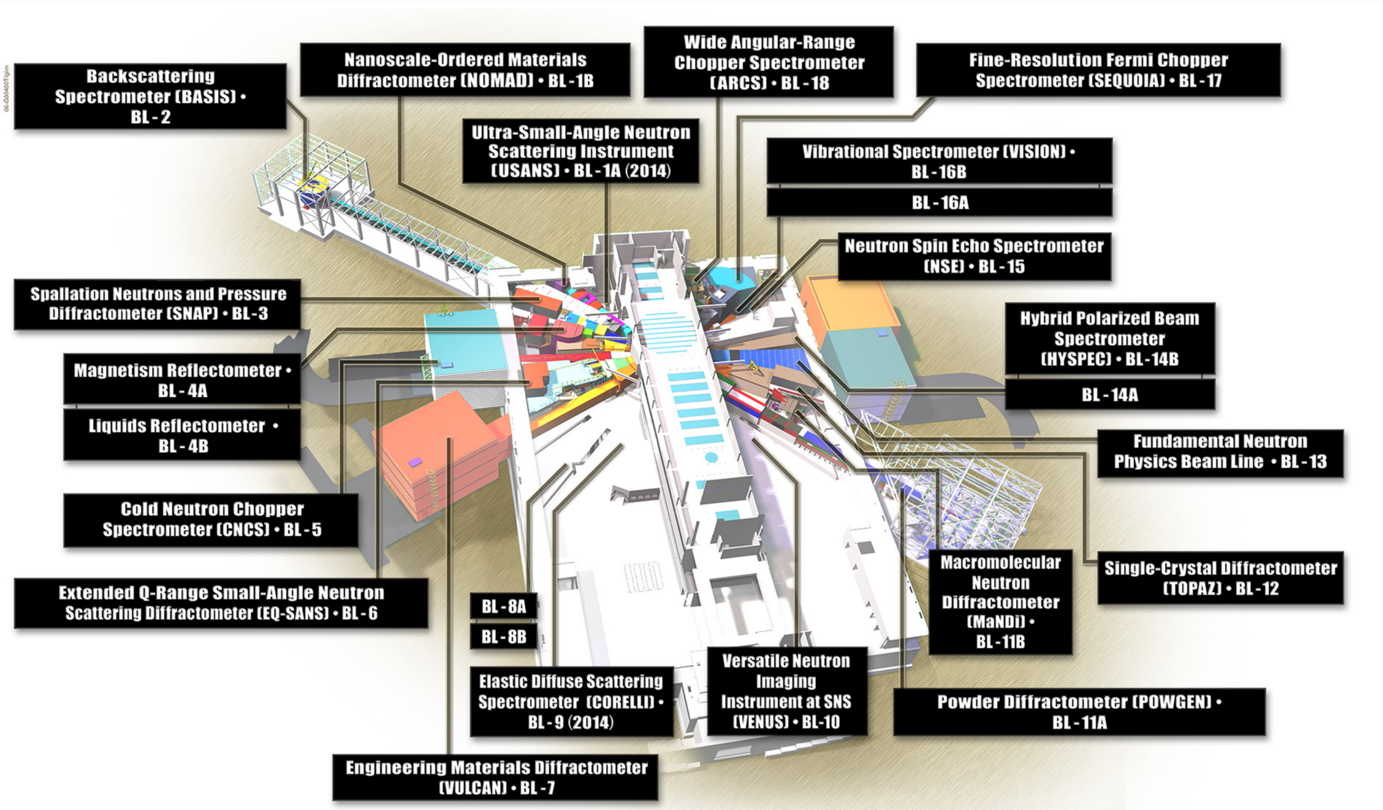
VENUS (BL-10): In engineered components, three-dimensional residual stress and strain mapping will reveal material and mechanical behaviors during operation and/or under exposure to extreme conditions such as heat and pressure. Supported in large part by the prospective user community, the new VENUS imaging beam line will provide the brightest source and highest energy resolution available for neutron imaging in the world.

VISION (BL-16B): Establishing appropriate sample environment equipment together with and the local availability of in situ photon probes such as Raman and/or IR spectroscopy will meet expressed requirements of a user community in chemical spectroscopy.

Appendix C: Instrument Layouts



The High Flux Isotope Reactor instrument layout.



The Spallation Neutron Source instrument layout.

Appendix D: Potential Expansion of Spallation Neutron Source Mission

The SNS accelerator mega-watt power level and GeV energy proton beam represents unique resources with a wide range of potential applications beyond neutron scattering. Currently, there is a fundamental neutron physics beam line for studying neutron decay, the hadronic weak interaction, and the search for a neutron electric dipole moment. A community of researchers in North America use muon spin rotation, relaxation, and resonance (muSR) in the study of materials; a pulsed source of muons would provide significant new capabilities. Spallation events produce copious amounts of mesons that stop in the target and decay at rest, resulting in the world's highest intensity pulsed source of low energy neutrinos. The high energy, high flux proton beam can also be the driver of an ideal simulator of the cosmic ray spectrum. A proposal for a fusion materials irradiation test station, which could be applied to targets at FTS, could be deployed in approximately three years. Other potential applications of the SNS proton beam include a source of fast neutrons for fast fission cross-section measurements, or isotope production using ~ 100MeV energy protons. There is a strong desire from the high energy and nuclear physics community for an ultra-cold neutron source. Longer-time-scale concepts include powering a third target station that could be used for applications such as large- volume samples, irradiation testing for fission and fusion materials damage testing, or an Isotope-Separation-On-Line capability for nuclear physics applications.

Appendix E: Potential Expansion of the High Flux Isotope Reactor Mission

HFIR's high power and very compact core make it an excellent source for neutrinos, which can be used for physics and nonproliferation research and development. The Neutron Sciences Directorate has been collaborating on several programs that would use HFIR as a neutrino source. Some of these would involve detector systems located in the HFIR reactor building, while others would require tunnel and cave facilities located about 0.5 km from the HFIR core.

A proposal to pursue a robust and flexible materials irradiation facility is under way. This would give researchers a means to actively control temperatures, pressures, and environments and, additionally, monitor experiments in situ. The proposed facility would provide flexible, cost-effective means for instrumented experiments, allowing not only for monitoring the samples themselves, but also for monitoring the effluent gases flowing from experiments. This opens the door to limited fuels testing and monitoring and research in the areas of gas release and uptake. This proposed facility is planned for completion in 2015.

HFIR was constructed with a critical pool to accommodate a future critical facility which was not built. This pool has been idle for many years and recently has been the subject of planning with the Southeast Universities Nuclear Reactors Institute for Science and Education to house a critical facility for nuclear research and education. A proposal is under way to develop this idea further with the goal of starting research in FY 2016.

An engineering design study of the conversion of HFIR from highly enriched uranium fuel to low enriched uranium (LEU) fuel is ongoing. Results to date indicate that conversion to LEU fuel requires an increase in reactor power from 85 MW to 100 MW to maintain the current performance of HFIR with respect to the neutron flux to the central target region, reflector, and beam tube locations.

Appendix F: Current Additional Missions of the High Flux Isotope Reactor

Isotope Production

Californium-252: HFIR supplies 70 percent of the world demand for californium-252, which is used as a reactor start-up source, in radiography for the coal and oil industry, and for medical therapy applications. The remainder is supplied by Russia. HFIR operation forms an irreplaceable cornerstone of this billion dollar industry.

Recently a new contract was signed between the DOE and the consortium of californium distributors extending the relationship an additional eight years. To meet customer demand, HFIR and the Radiochemical Engineering Development Center will execute californium campaigns roughly every two years. For HFIR, these campaigns involve irradiating up to 10 curium targets in the flux trap for up to seven HFIR operating cycles. Irradiations for the next campaign will begin January 2014 and extend into March of 2015.

Berkelium-249: In the pursuit of new elements on the periodic table, researchers from the United States and around the world rely on HFIR irradiations to produce berkelium-249 and other heavy element target material (e.g., Californium-251). Recent (2010) campaigns to produce berkelium-249 have resulted in the discovery of element 117, and use of these heavy element target materials continues in the search for elements 119+. This effort exemplifies fundamental scientific collaboration on an international scale.

Plutonium-238: The necessity for reliable power for the National Aeronautics and Space Administration's (NASA's) deep space and planetary missions drives the need for plutonium-238. Used in radio thermoelectric generators (RTGs), plutoinium-238 provides the most efficient heat source for these electricity-generating units and is the basis for the next generation Stirling engine generators, which are in NASA's development pipeline. The recent Mars rover, Curiosity, is powered by plutonium-238–driven RTGs.

In 2011, a program was initiated at ORNL, in conjunction with Idaho National Laboratory (INL) and LANL to develop the technology to produce plutonium-238 for NASA and other missions. In past decades, production of plutonium-238 required reactors at Savannah River National Laboratory, which are no longer operating This new program requires the use of both HFIR and the Advanced Test Reactor at INL for irradiations of neptunium-237 targets, which transmute into plutonium-238. Test irradiations have already begun at ORNL and will begin at ATR in 2015. Full-scale production is being planned for 2019.

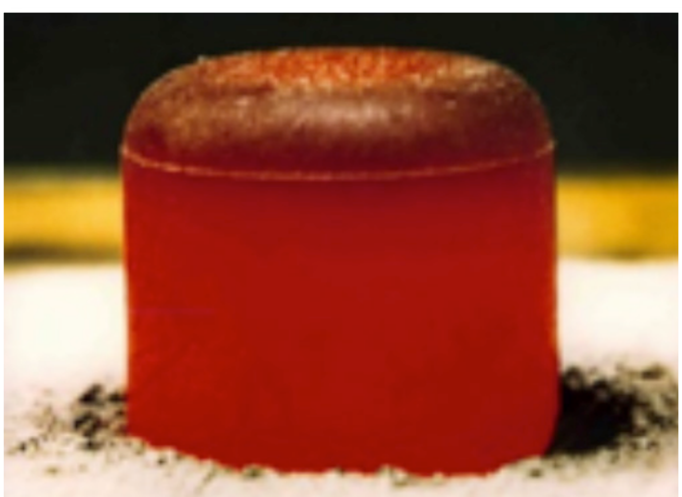


Image of a heated pellet of Pu-238.

Selenium-75: Used in commercial/industrial gamma radiography, selenium-75 is becoming the isotope of choice for many pipeline and other nondestructive testing efforts. HFIR's production of selenium-75 is increasing with the rising demand for this isotope. Additionally, the high specific activity only available from HFIR has become the industry standard.

Nickel-63: Because of the low target cross section, HFIR is the only source for high specific activity Nickel-63

Se-75 used for non- destructive examination of pipelines.

used for national security applications and detection of explosives and drugs at airports. A new campaign will begin in 2014 for irradiation of multiple targets to satisfy increasing demand for this isotope.

Materials Irradiation

HFIR offers a means for simulating 40 years of irradiation damage in mere months using 1.2×10^{15} n/cm^2-sec fast neutron flux. With very high neutron flux comes the ability to simulate the full life of radiation exposure for commercial reactor materials and components. Currently, HFIR contains roughly 100 separate experiment capsules and thousands of test specimens for various materials for the commercial nuclear power industry. These collaborations with DOE provide the necessary data for qualification of new reactor component materials, including nuclear fuel cladding and reactor vessel materials.

Whether for materials tests for a nuclear reactor on the moon or for research of radiation effects on artificial spinal disc materials, the gamma irradiation facility at HFIR offers a uniquely high dose rate by using the HFIR spent fuel as a gamma source. Selecting older spent fuel allows the selection of lower dose rates, and the ability to run electrical and gas lines to the sample chamber allows “live” testing of electrical equipment, heated samples, and various gas environments. Additionally, unlike cobalt-60 gamma sources, the HFIR facility provides a full spectrum of gamma ray energies.

Neutron Activation Analysis

Neutron activation analysis (NAA) offers a combination of ultrasensitive measurements and fast turnaround for determining the presence of certain elements in a material. The NAA Laboratory at HFIR provides irradiation and detection services for a wide variety of programs. These include research on material impurities, understanding the nature and quantity of pollution in the environment, qualifying ultrapure materials used in highly sensitive detectors, and detection of trace quantities of nuclear materials. The NAA Laboratory participates in the International Atomic Energy Agency (IAEA), Pre-Inspection Check program, irradiating and testing between 30 and 100 samples submitted by IAEA inspectors.

In the world of NAA, high neutron flux translates directly to increased detection sensitivity. The high thermal flux available to the NAA Laboratory allows the detection of isotopes that no other research reactor in the United States can generate in measurable quantities. The ability to measure more isotopes means that more materials can be analyzed for forensic research.

The ability to irradiate in a very high flux and use delayed neutron counter technology allows researchers at ORNL to detect low PPT (parts per trillion) quantities of uranium-235 and plutonium-239. This provides a nuclear forensics capability that cannot be duplicated anywhere else in the world. Additionally, there is currently research into the deconvolution of decay curves for simultaneous determination of uranium-235 and plutonium-239 using delayed neutron counting. If successful, this could offer a revolutionary capability to nonproliferation programs.

Acronyms

ADARA: Accelerating Data Acquisition Reduction and Analysis

APS: Advanced Photon Source

ASCR: Advanced Scientific Computing Research

ATR: Advanced Test Reactor

BER: Office of Biology and Environmental Research

BES: Office of Basic Energy Sciences

BESAC: Basic Energy Sciences Advisory Committee

BESC: BioEnergy Science Center

CAMM: Center for Accelerating Materials Modeling

CCSD: Computing and Computational Sciences Directorate

CD: Conceptual Design

CNCS: Cold Neutron Chopper Spectrometer

CNMS: Center for Nanophase Materials Sciences

CSMB: Center for Structural Molecular Biology

ESS: European Spallation Source

DOC: Department of Commerce

DOE: US Department of Energy

EFRC: Energy Frontier Research Centers

FIRST: Fluid Interface Relations, Structure and Transport

FTS: First Target Station

FY: fiscal year

HEU: Highly enriched uranium

HFIR: High Flux Isotope Reactor

IAEA: International Atomic Energy Agency

ICND: International Collaboration on Neutron Detector Development

INL: Idaho National Laboratory

IRP: Inner reflector plug

J-PARC: Japan Proton Accelerator Research Complex

JSNS: Japan Spallation Neutron Source

LANL: Los Alamos National Laboratory

LENS: Low Energy Neutron Source

LEU: low enriched uranium

MD: Molecular Dynamics

MIEZE: Modulated Intensity by Zero Effort

MIF: Materials Irradiation Facility

NAA: Neutron Activation Analysis

NAB: Neutron Advisory Board

NAS: National Academy of Sciences

NCNR: NIST Center for Neutron Research

NDT: Nondestructive testing

NIH: National Institutes of Health

NIST: National Institute of Standards and Technology

NMR: Nuclear Magnetic Resonance

NScD: Neutron Sciences Directorate

NSE: Neutron Spin Echo

NSF: National Science Foundation

OLCF: Oak Ridge Leadership Computing Facility

ORNL: Oak Ridge National Laboratory

PPT: Parts Per Trillion

REDC: Radiochemical Engineering Development Center

RF: Radio-frequency

RH: Relative Humidity

RTG: Radio Thermoelectric Generators

SANS: Small Angle Neutron Scattering

SBIR: Small Business Innovation Research

SERGIS: Spin Echo Resolved Grazing Incidence Scattering

SESANS: Spin Echo Small Angle Neutron Scattering

SHaRE: Shared Research Equipment Collaborative Research Center

SING: SNS Instruments Next Generation

SNS: Spallation Neutron Source

SRL: Savannah River Laboratories

STS: Second Target Station

STTR: Small Business Technology Transfer

TAS: Triple-axis spectrometers

TDR: Technical Design Report

TOF: Time-of-Flight

US: United States

USANS: Ultra-small Angle Neutron Scattering

USDA: US Department of Agriculture

VI: Virtual Institute

WAND: Wide Angle Neutron Diffractometer

WANS: Wide Angle Neutron Scattering

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