Instruments for Emerging Science: A Science Case for the Second Target Station

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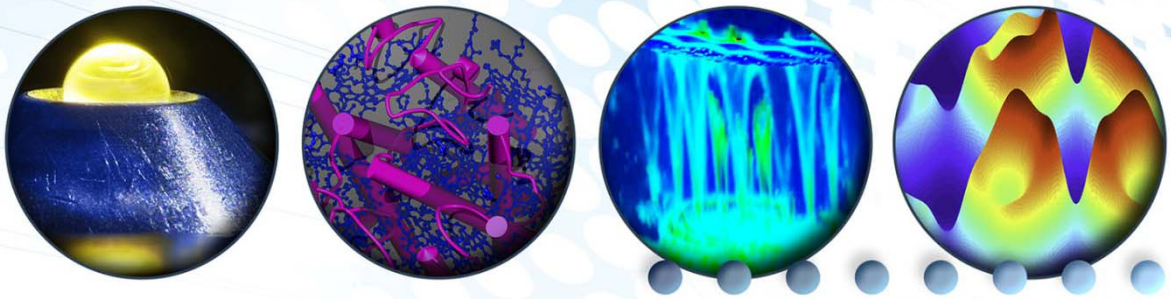

OAK RIDGE National Laboratory

1. INTRODUCTION

Oak Ridge National Laboratory (ORNL) is a leading center for neutron sciences worldwide with the mission to ensure that the nation is served with cutting-edge capabilities for undertaking research that addresses the needs of the Department of Energy as well as the broader community. As part of this mission, the Neutron Sciences Directorate (NScD) has undertaken, in consultation with the sponsors and science community, an in-depth look at the major needs for neutron sciences and areas of significant impact spanning the next decade and beyond. A central part of this process has been the formation of four high level science-themed workshops to delineate emerging and future challenges and identify priority areas where developments in neutron sciences are most needed. This effort has been complemented by the formation of a series of working groups charged with exploring how these challenges could be addressed. A key component is the proposed Second Target Station (STS) at the Spallation Neutron Source (SNS), which will create new opportunities for neutron sciences as the first Fourth Generation Neutron Source (see Fig. 1.1).

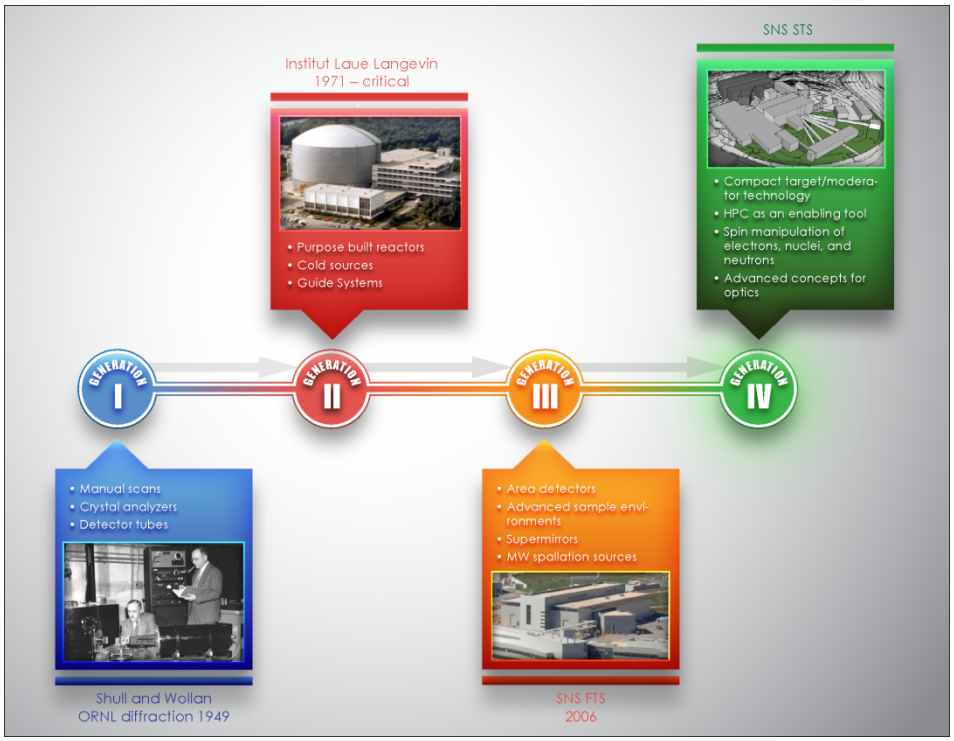

Fig. 1.1. Converging source and instrumentation technologies have defined completely new scientific capabilities with each generation of neutron facility. The Institut Laue-Langevin (ILL) in France integrated the technologies of the day into a class defining facility. Over the years, many of the advances of the technologies of Generation III have been integrated into this facility, especially with the Millennium project, and ILL remains one of the leading neutron facilities worldwide. In the United States, the construction of SNS brought a new level of capabilities in the form of a mega-Watt pulsed spallation source that re-established ORNL as a leading center. Second Target Station will, along with the planned European Spallation Source, be among the first fourth generation neutron facilities worldwide and will open up new areas of science.

STS was recognized as being "absolutely central" to US science in the Office of Science Facilities Prioritization Round 2013. However, there were "science/engineering challenges to resolve before initiating construction." The engineering challenges are largely assessed in the accompanying Technical Design Report (TDR) documentation, while the following scientific challenges are addressed here:

(1) What are the expected needs for neutrons and requirements for instrumentation?

(2) Where do neutrons fit in with other developments in photons, electrons, etc., and where will they remain irreplaceable?

(3) What new scientific capabilities can STS deliver?

(4) How would a Second Target Station complement the capabilities of the First Target Station at SNS and the High Flux Isotope Reactor (HFIR)?

1.1 FUTURE SCIENCE NEEDS FOR NEUTRONS AND THEIR ROLE

To identify emerging science where neutrons are an essential tool as well as the needs of the community, four workshops addressed the future of quantum condensed matter, soft matter, biology, and the frontiers in materials discovery. These workshops provided a host of compelling scientific and technological challenges for the decade ahead that are inaccessible to other techniques or where the contribution of neutrons in combination with other techniques is vital. They also identified areas where a step change in capabilities is needed. In nearly all cases, the primary capability gaps that need to be addressed require more intense beams in the long wavelength ("cold") regime and for instrumentation using a large bandwidth. STS, as proposed in the accompanying TDR[1], will provide exactly these capabilities and will be the most advanced source of its kind. Indeed, the capabilities envisaged will make this a truly next generation facility, and together with the first target station and HFIR reactor source, the STS facility will ensure US capabilities that go beyond any existing or planned sources worldwide for the next generation.

1.1.1 Quantum Materials[2]

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

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

[1] "Second Target Station at the Spallation Neutron Source" Technical Design Review, October 2014.
[2] Based on the report of the Quantum Condensed Matter Workshop, December 5–6, 2013, LBNL, Bob Birgeneau, UC Berkeley.

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

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

A major trend in the coming years is the increasing importance of mesoscale phenomena for controlling properties. These techniques will require spatially-resolved probes of (especially magnetic) structure of materials on the sub-micron scale, as well as determination of the structure of partially ordered materials including defect structures (Fig. 1.2).

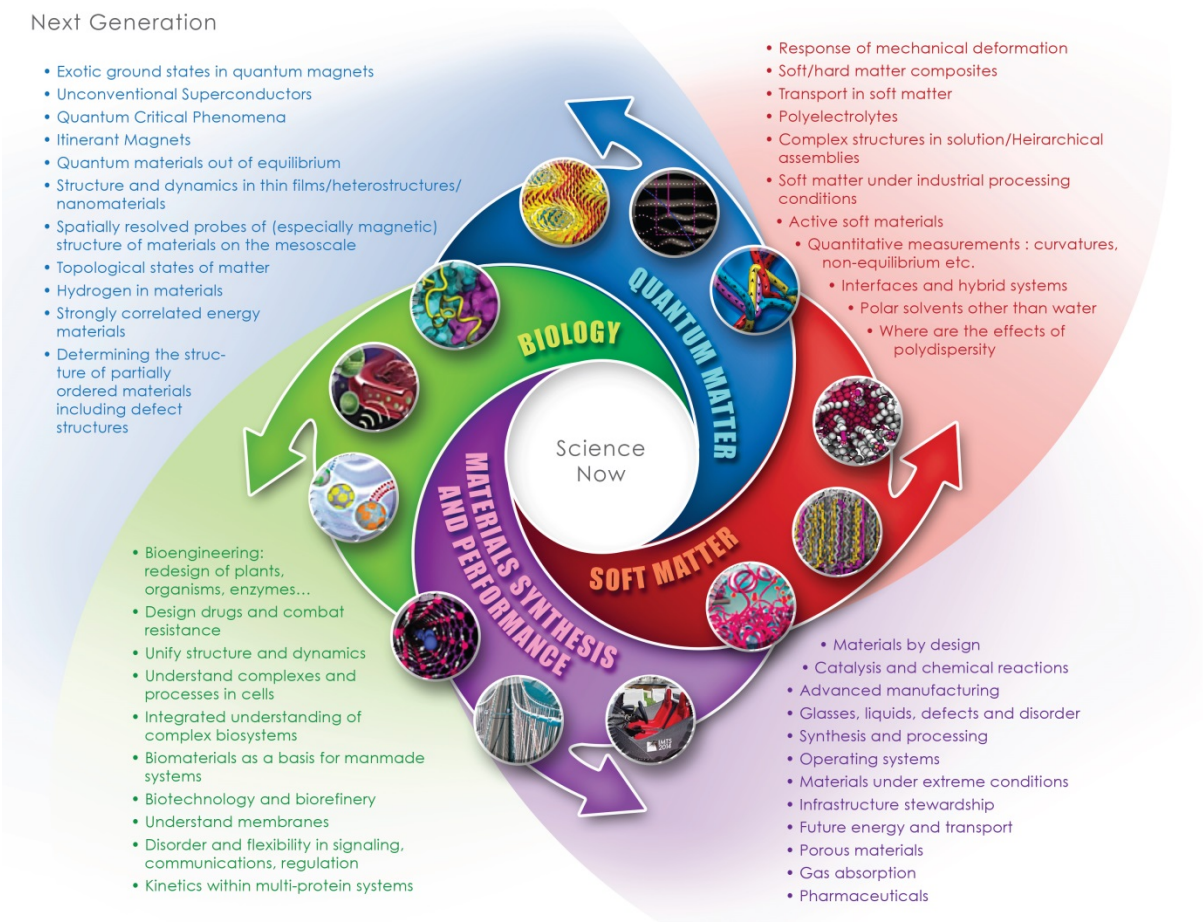

Fig. 1.2. Neutrons are either unique or play a vital role in combination with other experimental techniques over an enormous range of next generation science challenges. Shown above are key areas identified in the workshops where neutrons are needed but also require new capabilities. What these capabilities could look like is developed in this document.

The new challenges identified here need the much more advanced capabilities in cold neutrons offered by STS. Focused beams will be required to measure smaller samples, and the technology to fully exploit polarized beams is necessary to separate the component parts of complex states in materials. Coupling neutrons with materials exploration requires more versatile measurement capabilities, including application of multiple characterization techniques. Furthermore, the manipulation of states in situ means enhanced sample environments are crucial. Neutrons are unparalleled in their direct relevance to theory, and the most advanced data analysis and simulation capabilities are needed to address this potential.

1.1.2 Soft Matter[3]

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

Areas of compelling scientific need where neutrons will play a key role have been established. These extend into the response of soft matter to mechanical deformation, soft/hard composite materials, interfaces, and transport in soft matter. Also of fundamental need are capabilities to understand polar solvents other than water, polyelectrolytes, and complex structures in solution such as hierarchical assemblies. The widespread impact of soft matter technologies will require looking at soft matter under industrial processing conditions, understanding active soft materials, expanding our ability to make quantitative measurements, and gaining insight into the effects of poly-dispersity on physical properties.

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

1.1.3 Biology[4]

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

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[3] Report from "Grand Challenges in Soft Matter" workshop May 17–18, 2014, University of California Santa Barbara, Fyl Pincus (UCSB) and Matt Tirrell (University of Chicago).

[4] Report from "Grand Challenges in Biological Neutron Scattering" workshop January 17–18, 2014, University of California San Diego, Susan Taylor (UCSD) and Heidi Hamm (Vanderbilt University).

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

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

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

1.1.4 Materials Discovery, Characterization, and Application[5]

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

The unique physical properties of neutrons make high intensity beams indispensable to materials discovery, characterization, and application where they complement the capabilities of electrons and photons. Among these characteristics, their nondestructive nature, ability to penetrate real components and materials under working condition, sensitivity to light elements, ability to observe modes and dynamics over virtually all length and time scales, absence of selection rules, and the ability to highlight

[5] Report from "Frontiers in Materials Discover, Characterization, and Application" workshop August 2–3, 2014, Schaumburg, IL, George Crabtree (Argonne National Laboratory) and John Parise (University of Stony Brook).

components using isotope substitution make their contribution unique. Areas where neutrons will be essential for future materials science and engineering include infrastructure stewardship, advanced propulsion systems, advanced materials processing, nuclear fuels and radiation tolerant materials, energy storage and energy conversion integrated systems, materials by design (integrated computational materials engineering), and materials under extreme environments.

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

1. Monitoring and understanding chemical reactions and catalysis including gas adsorption and separation

2. Using analytical chemical spectroscopy where neutrons could provide a high throughput technique, providing information not accessible to photons

3. Understanding the role of disorder and defects and manipulating these

4. Addressing the fundamental challenges of glasses and liquids as well as fluid flow and reactivity

5. Conducting in situ studies including under pumping conditions, kinetics studies, materials growth and synthesis, and materials under extreme conditions

6. Understanding how components and integrated materials in devices function under realistic conditions using instruments that can combine multiple techniques such as imaging, diffraction and spectroscopy

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

Overall, the outstanding scope of the science and technological challenges where neutrons play an irreplaceable role ensure they will be needed as a central part of a national facilities strategy for decades to come and show the compelling need for forefront facilities to ensure scientific and technological competitiveness.

1.2 ADDRESSING FUTURE SCIENCE CHALLENGES WITH SECOND TARGET STATION

To connect these science challenges with the source capabilities provided by STS and determine how this would be complemented by the First Target Station and HFIR, we convened a series of 14 working groups involving 70 of our scientists (Fig. 1.3). They were charged with exploring new concepts and instrumentation. In this report we present a series of instrument concepts that demonstrate new levels of performance as well as proposed science these instruments would allow that we cannot do now. Together, these new concepts provide a case for the impact of neutrons for the coming decade and beyond and demonstrate the compelling need for a Second Target Station at the Spallation Neutron Source.

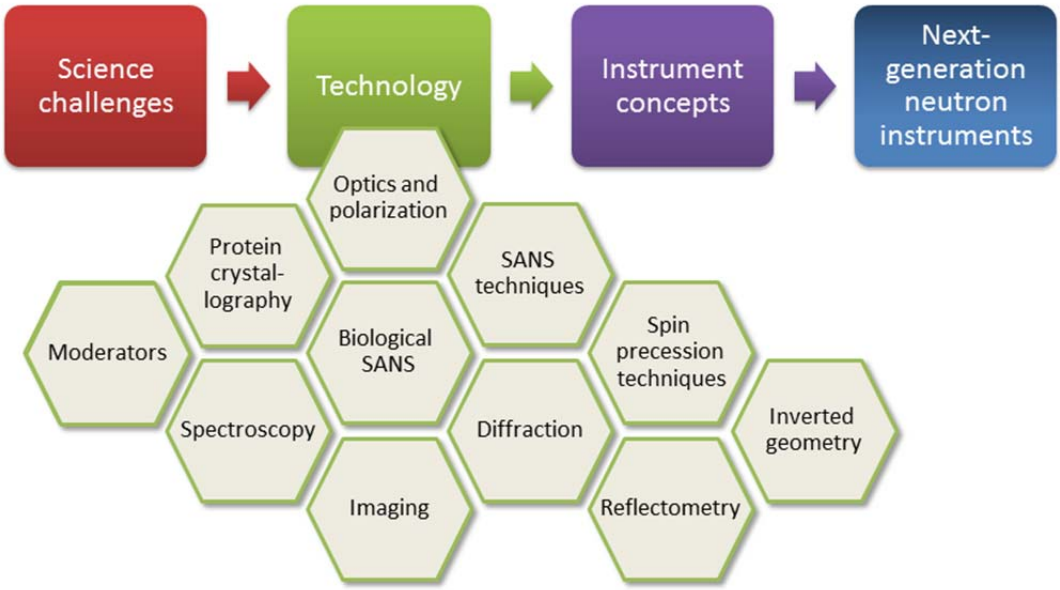

Fig. 1.3. The working groups were charge to explore transformational performance changes that would access new science.
The groups were formed from experts in science, technologies, and instrumentation. By exploring fundamental physical limits, new ideas for instrument types were generated.

1.3 PERFORMANCE AND CAPABILITIES OF SECOND TARGET STATION: A FOURTH GENERATION NEUTRON FACILITY

As outlined in this document, the performance and capabilities of the instrumentation enabled by STS make it truly a next generation facility (Fig. 1.4). Gains in performance of two orders of magnitude and beyond over existing capabilities make it transformative for many of the compelling research areas identified. At the heart of this dramatic step forward in capabilities are a series of advances that, when combined, create new classes of instrumentation. The major drivers for this advancement include, of course, the advances in target and moderator technology (see TDR), as well as high performance computing that enables reconstruction and analysis of multimodal data and simulation of systems gluing together disparate data sets and open complex scenarios to analysis and interpretation. In addition, the big advances in manipulation of the spin of electrons, nuclei, and neutrons allow control of scattering cross sections and contrast in situ and revolutionize what we can measure in magnetic and hydrogenous materials. Another area of great advance is in neutron optics where lensing, guiding, and wavelength analysis are all taking major steps forward. Taken together these define STS as a new generation of neutron facility of far reaching science impact.

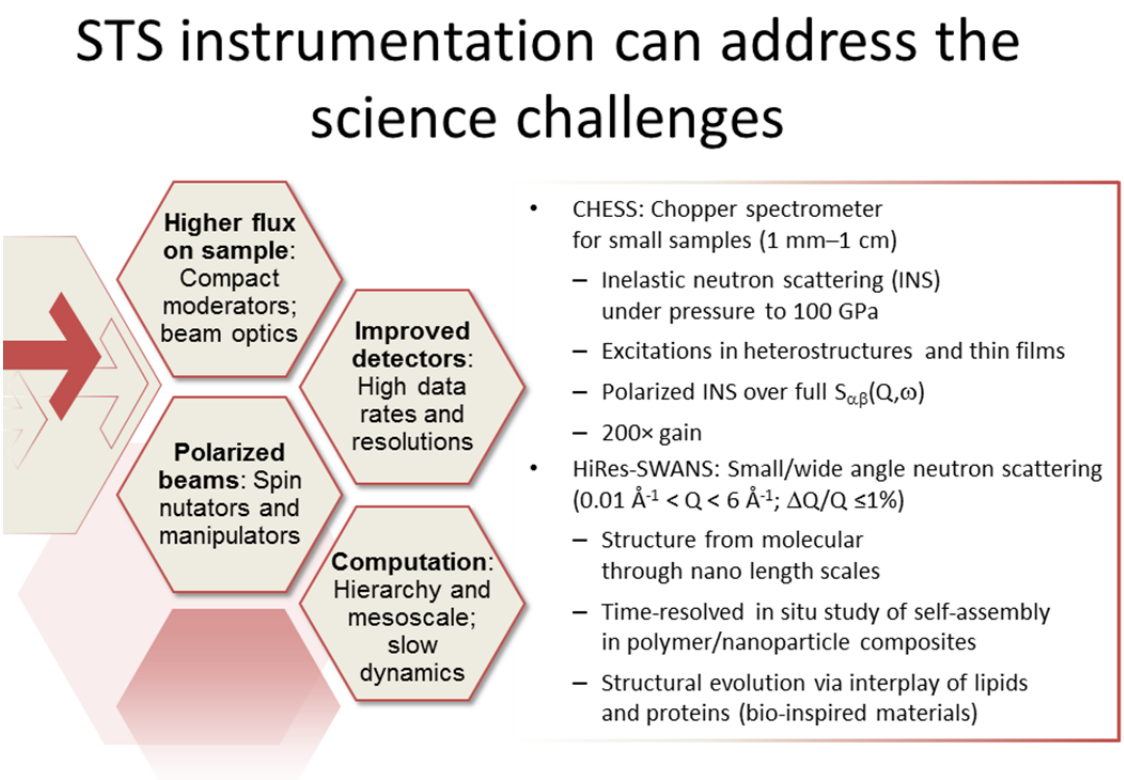

Fig. 1.4. The convergence of technologies in source and moderators, high performance computing, spin manipulation, and optics allows new levels of performance.
These include transformational advances in spectroscopy. An example is the CHESS instrument, which will achieve gains of 200 over the current world leader CNCS at SNS. This advancement opens up the ability to look at dynamics in artificial crystals grown by epitaxy as well as heterostructures bringing neutrons to new realms of quantum materials and devices. Hierarchical materials present challenges beyond anything available currently. The HiRes-SWANS concept combines small and wide angle scattering to span length scales, giving access to structure from chemical bonding to mesoscale organization. This new class of instrumentation enabled by source and optics will be crucial for understanding the functional materials of tomorrow.

1.4 SCIENCE IMPACT OF SECOND TARGET STATION

We have explored 22 instrument concepts for the Second Target Station, which provide unprecedented levels of performance (See Fig. 1.5). These offer multimodal measurements both in terms of using advanced optics and computing to allow measurement and integration of multiple types of neutron measurement simultaneously but also enabling orthogonal, complementary techniques to monitor the system in parallel. In addition, the flexibility of design offered by new manufacturing technologies and complex data handling will allow the concept of a laboratory on a beam line to be realized where steering of complex interactive experiments is made in real time and in situ/in operando conditions can be designed as an integral part of the beam line from the beginning of operation.

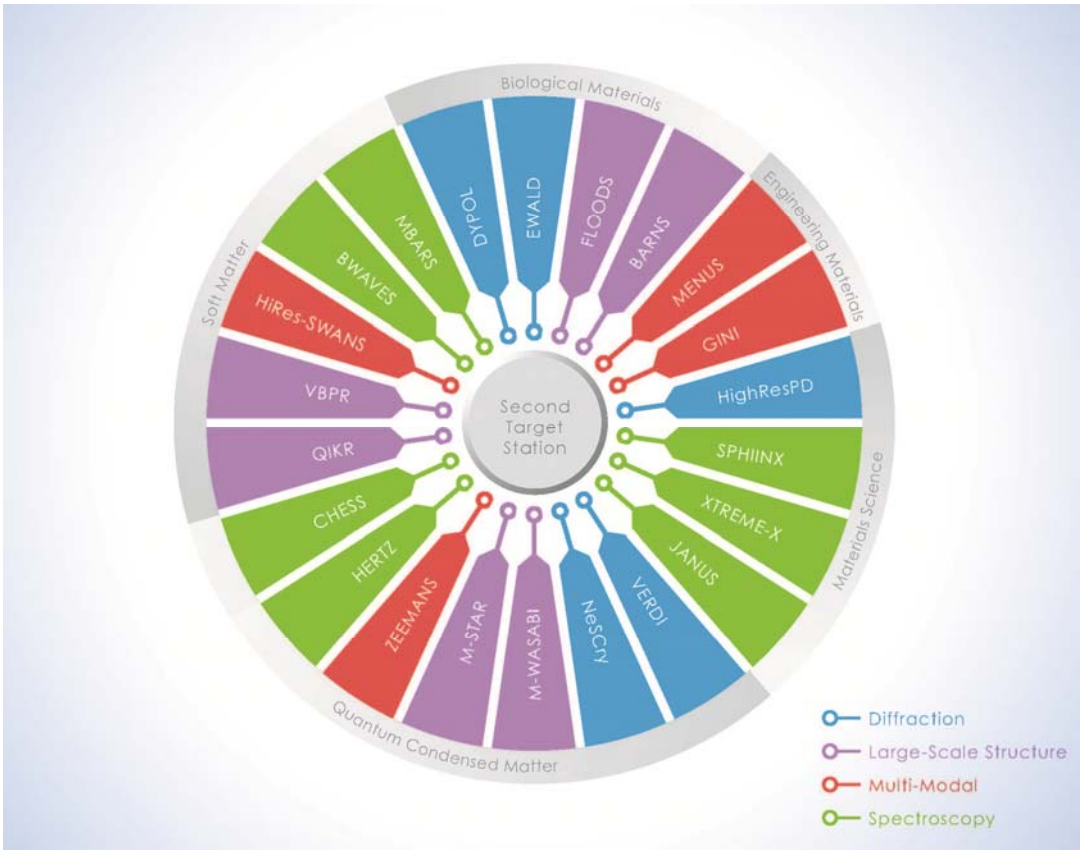

Fig. 1.5. The 22 neutron scattering instrument concepts explored for the Second Target Station span a range of science capabilities and science areas.

Overall, the development of the Second Target Station will ensure the US lead in neutron sciences for the foreseeable future. It will impact our understanding of materials by giving an integrated understanding from the atomic to real world scales. It will provide unprecedented access to mesoscale quantum and complex matter and ensure that the unique contributions of neutrons to discovery and understanding in these fields continue for decades ahead. The advent of 3D mapping and micro-spot technologies as well as the source intensity and novel instrumentation allow in situ and in operando studies, not just of exemplary materials but also of real operating systems, in the most challenging problems in technology and engineering. Automation and high throughput instrumentation, coupled with advanced modeling, databases and libraries, will put STS center stage coupling big data with computational resources to enable predictive control and design of materials. Already, the close relation between theory and experiment is putting neutrons at the forefront of the revolution in combining simulation and data. The high intensity beams and advanced handling capabilities will bring new insights into kinetics, out of equilibrium, and chemical reactions. They will facilitate not just the understanding of materials but also their synthesis and impact of processing conditions. Such capabilities, we predict, will become all the more important as the prediction of compelling material compositions makes advances in their synthesis all the more pressing. Finally, the major step forward in capabilities possible with STS will reach out into new science areas and bring whole areas of science, like biology and materials chemistry, into reach where the unique properties of neutrons can then play as important a role as they do today for quantum condensed matter and soft materials (Fig. 1.6).

Fig. 1.6. The second target station and instrumentation in this report provide transformative science capabilities impacting materials challenges and the new ways in which research is undertaken.

1.5 THREE SOURCE STRATEGY

STS will provide the means to address many of the outstanding challenges identified in the workshops, but neutron scattering techniques that are best optimized to different source characteristics are also a key requirement. The cold neutron beams and long repetition rate of STS perfectly complement the SNS First Target Station and HFIR. Together these facilities form an unbeatable combination that will give the United States clear leadership in neutron science capabilities for the next 20 years and beyond, allowing it to match or go beyond the capabilities of all existing or planned facilities worldwide. As part of our optimization strategy, we have explored instrument concepts at HFIR and FTS that can also take advantage of the advances detailed above to address the challenges identified in the science workshops. These new instrument concepts are also described in this document as part of a coherent approach to delivering an unparalleled and integrated set of neutron science capabilities. Figure 1.7 below summarizes the role of each facility and its strengths and the instrumentation types.

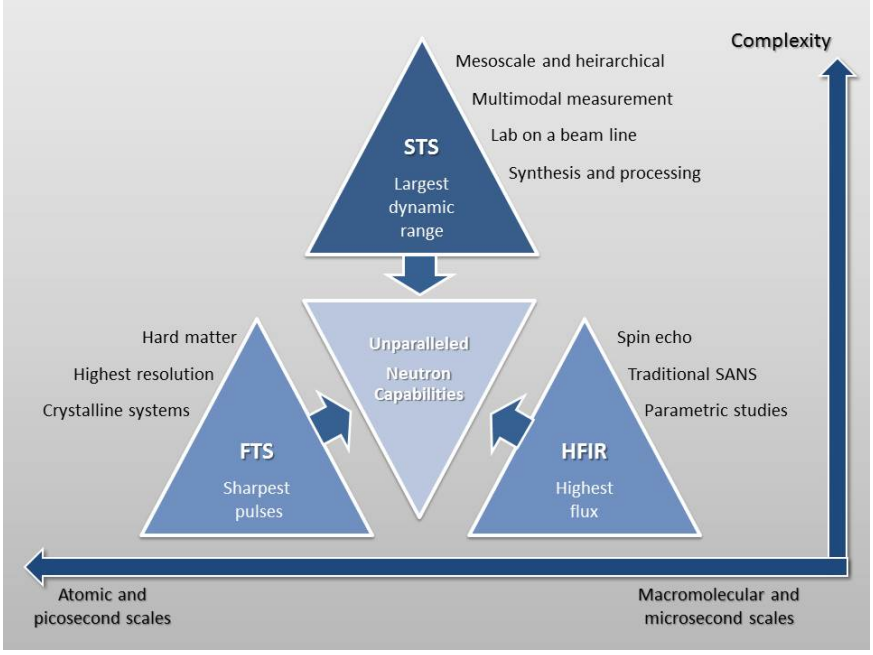

Fig. 1.7. The ORNL three source strategy.

1.6 FUTURE STEPS

The instrument concepts presented in this report are just a start. There are new instrument ideas and compelling science questions in the community that have not yet been explored. To access the creativity and collective wisdom of the whole US science community, we will hold a series of workshops to build on and add to the ideas presented in this document and continue the dialog about the role that neutrons will take in addressing the science challenges of today and the next decades. In addition, ORNL is investing directly in challenge experiments designed to demonstrate the capabilities that will be routinely available at STS for addressing the science of tomorrow. These experiments will use nuclear spin manipulation to transform the measurement of biosystems, establish infrastructure leading to inelastic measurements at extreme pressures of 40 GPa and above, and develop our strategy for simultaneous structural characterization of hierarchical materials over the broadest range of length scales. This is an exciting time for neutrons, and we hope you enjoy reading the report and encourage you to get involved in defining the future of neutron scattering in the United States.

1.7 CURRENT AND PROPOSED NEUTRON SOURCES AT ORNL

K. W. Herwig (ISD)

1.7.1 Introduction

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

in technologies and techniques, will add science capabilities and increase capacity over the next five years.

The 1998 report of the Russell Subpanel [1] defining the technical specifications for SNS included recommendations to design the facility "such that it can be operated at a significantly higher power in a later stage" and to include the "capability of additional targets." Both of these recommendations were incorporated into the original SNS design. The mission need for a SNS Second Target Station (STS) has been recognized by the Department of Energy with approval of CD-0 in January 2009 to "provide an additional target station at ORNL optimized for cold neutron beams." Appendix A provides an abbreviated discussion on relative merits of the technical design requirements of STS. The current STS concept is a short-proton pulse, 10 Hz facility optimized for high peak-brightness, long-wavelength neutron pulses produced by coupled moderators. However, a number of the instrument concepts in the following sections propose taking full advantage of the 10 Hz STS operating frequency but require the sharper neutron pulses provided by a de-coupled, poisoned moderator. Current neutronics calculations indicate that such a moderator can be supported with minimal impact on the coupled moderators.

1.7.2 Source Characteristics and Strengths

HFIR

The HFIR cold-source is comparable to the world's best reactor sources and provides the highest time averaged cold neutron flux of the ORNL sources, approximately 10× that of the proposed SNS STS as shown in Fig. 1.8 (a). In addition, HFIR produces approximately 40× the time-averaged thermal neutron flux of the SNS First Target Station (FTS).

The guide system delivering neutron beams to the cold instruments in the HFIR guide hall was designed in 1999 and started neutron beam operations in 2006. There have been major advances in neutron guide technology and neutron optics design in the past 15 years which have prompted an assessment of the HFIR neutron guide system. Section 6.3 provides a short description of a new guide concept for the HFIR cold source that would provide additional instrument end stations and improve neutron beam delivery for current instruments. Several of the proposed instrument concepts in the following sections would be supported by this new guide system.

SNS First Target Station

The SNS FTS is optimized for producing the highest wavelength resolution across a wide neutron spectrum. The two de-coupled, poisoned moderators that produce the shortest time neutron pulses and illuminate two-thirds of the SNS FTS neutron scattering instruments are placed in the most favorable positions relative to the Hg target. The two coupled H_2 moderators provide high fluxes of cold neutrons but have much broader time pulses than the de-coupled moderators and are placed in less optimum positions relative to the target, which limits their performance relative to the total number of neutrons they produce. Figure 1.8 (b) compares the pulse widths for the SNS moderators. FTS produces neutron

pulses at 60 Hz. The current STS project includes a doubling of the accelerator proton power from 1.4 MW to 2.8 MW with 2 MW available to FTS. The neutron scattering instruments and target shielding have all been designed for 2 MW operation, although some target modifications are likely needed because of the increased heat load. The current STS plan calls for operating the two sources in "pulse stealing" mode with five out of six pulses directed to FTS, and the remaining pulse directed to STS. One out of five of the FTS pulses will provide a longer counting time (broader wavelength band as discussed below) because of the missing pulse, but this will be of limited use because the choppers that define this band width cannot be re-set rapidly enough. The chopper systems on FTS will continue to operate as it currently operates, but with one pulse missing out of every 6.

SNS Second Target Station

STS is optimized for the highest cold neutron peak brightness, as shown in Fig. 1.8 (c). (Peak brightness is essentially the amplitude at the peak of the neutron time pulse emitted by the moderator as shown in Fig. 1.9.) In complementary fashion to FTS, coupled moderators will be placed in the most favorable positions relative to the target, maximizing their neutron production. Nonetheless, a number of the proposed instrument concepts require a much lower operating frequency than FTS but also require the sharp pulses of the decoupled moderators and would be well-served by the 10 Hz STS. The current STS concept includes three moderators: two coupled moderators of different geometry that are placed in the most favorable locations and a de-coupled moderator illuminating the remaining beam lines. Figure 1.9 shows pulse shapes at select wavelengths for the coupled moderators on both FTS and STS. Reducing the STS moderator dimensions to 3 × 3 cm^2 will

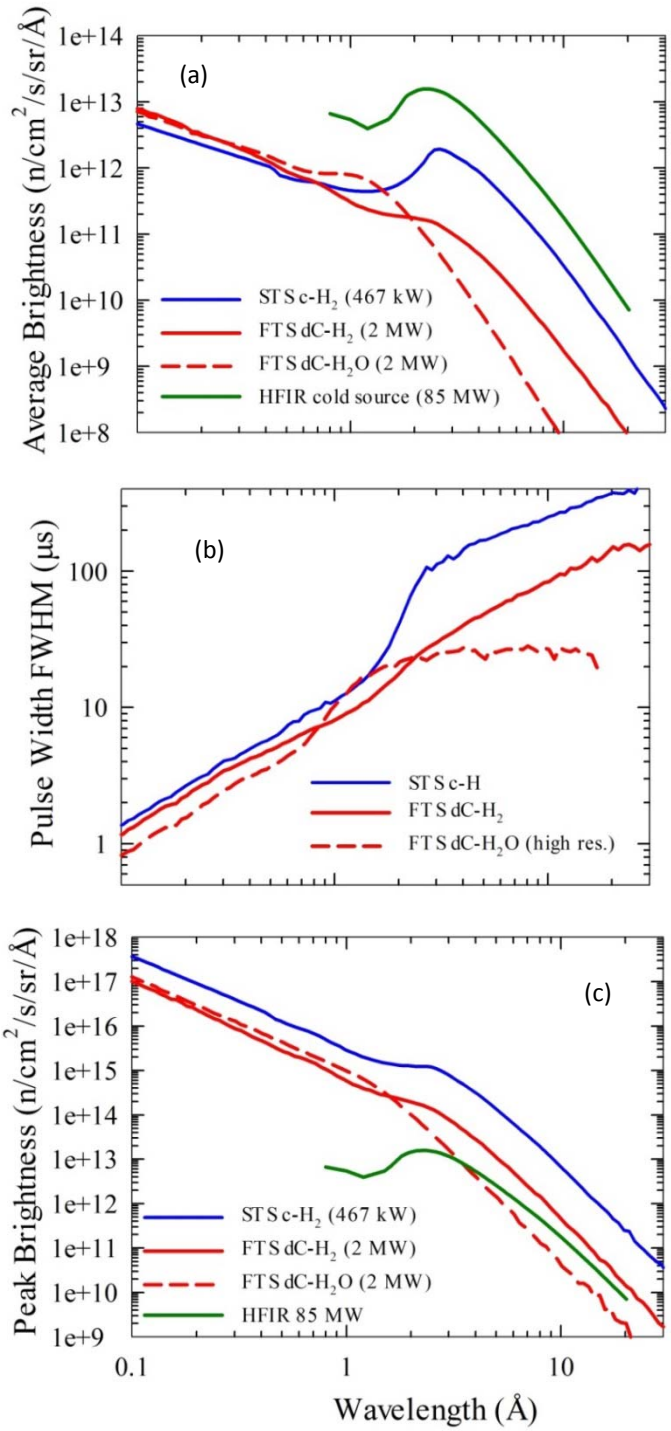

Fig. 1.8. Comparison of ORNL neutron source characteristics.
(a) Time-averaged brightness of ORNL neutron sources. The SNS de-coupled and coupled moderators are shown for FTS and STS, respectively. These are the moderators for which the source was optimized. (b) Moderator pulse widths for the FTS de-coupled moderators and the STS coupled moderator. (c) Peak neutron brightness.

improve the peak brightness by an additional factor of ~2 relative to the 10 × 10 cm^2 moderator.

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

1.7.3 Optimizing Instruments at Three ORNL Neutron Sources

The operating frequency, *f*, 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 *f* and the length, *d* (m), of the instrument, $\Delta\lambda = 3956/(d \cdot f)$. Higher source operating frequencies favor shorter instruments or instruments that use a small Δλ. For elastic techniques, the gains in employing time-of-flight (TOF) techniques are proportional to the number of useful instrument resolution elements available within this wavelength band. Consider the case of a high resolution powder diffractometer with a wavelength resolution $\delta\lambda/\lambda$ = 0.0005 and a desire to use wavelengths from 0.5 to 6.0 Å to obtain a complete data set. Such an instrument uses ~5,000 resolution elements and has the possibility for a TOF gain of 5,000 if all these elements can be obtained within a single pulse of the neutron source. If multiple pulses are required, the TOF gain is diminished accordingly. 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.

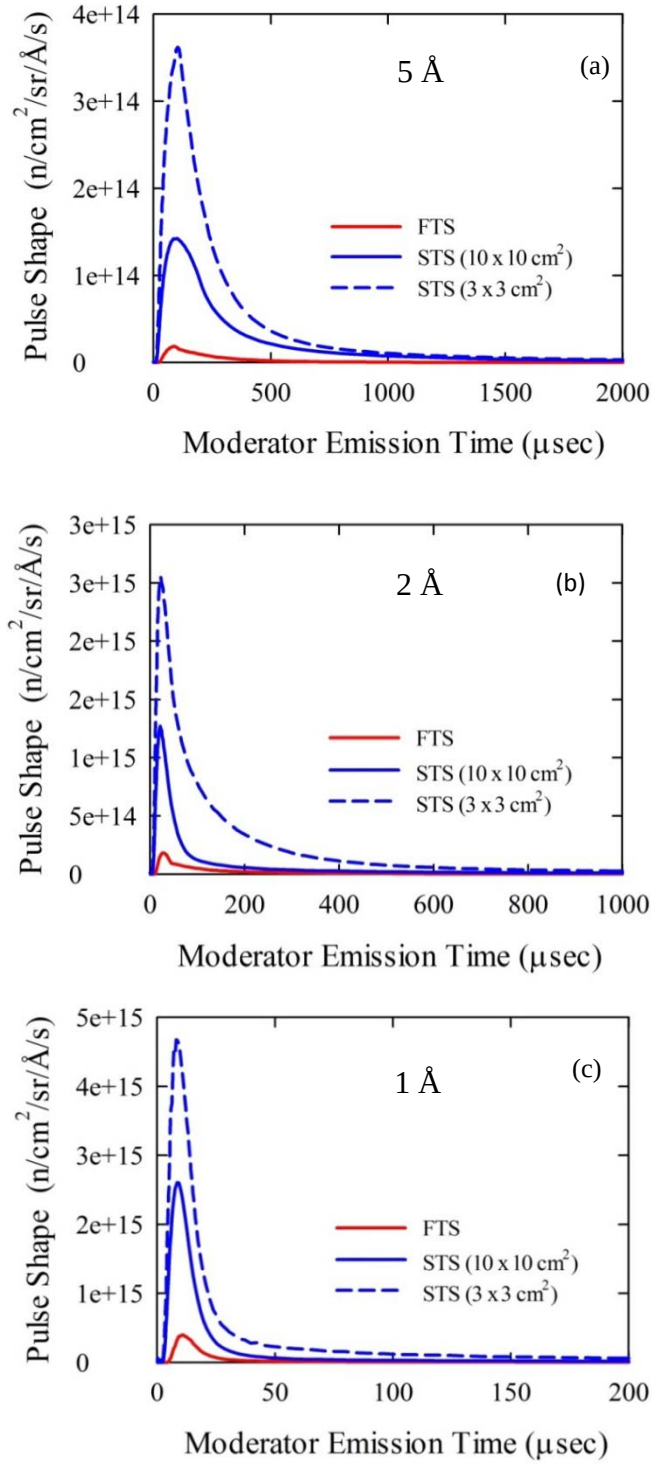

Fig. 1.9. Moderator pulse shapes for coupled moderators at FTS and STS at λ = 5 Å, 2 Å, and 1 Å in (a), (b), and (c) respectively.
Note that the time scale is changing in each plot.

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

Figure 1.10 is an optimal performance map of elastic scattering techniques across ORNL neutron sources showing nominal ranges for many neutron scattering instrument types. 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 Fig. 1.10 is the desired wavelength resolution expressed as $\delta\lambda/\lambda$. The y-axis is the number of these wavelength resolution elements required for any given measurement as discussed above and also represents the gain that an instrument can achieve from using TOF techniques. 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 $(\delta\lambda/\lambda)^{-1}$ and is indicated by the dashed line. Within the labeled boxes, we expect the performance of the indicated pulsed source to exceed that of HFIR; outside the boxes, HFIR will obtain a desired set of data more quickly. That is, the gains from using TOF exceed the difference in time-averaged flux between the pulsed sources and HFIR. 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 the 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 $\delta\lambda/\lambda$ of 1%, STS can potentially measure a given sample as quickly as HFIR, provided more than 10 resolution elements are required to complete a data set. If 100 resolution elements are required, STS could potentially make a measurement 10 times faster than HFIR. Whereas there is a region in which FTS and STS overlap, there are also regions where each excels. The same conclusion applies to a comparison of HFIR with either pulsed source. The boxes for the pulsed sources are constructed for the moderator types they were optimized for—FTS: de-coupled, poisoned; and STS: coupled. The vertical and diagonal boundaries of the boxes are set by the maximum and minimum possible instrument lengths, 100 m and 15 m, respectively. (Although one or two instruments could be placed as far as 120 m from the moderator at STS, the majority must be located within ~90 m given restrictions on the site geometry.)

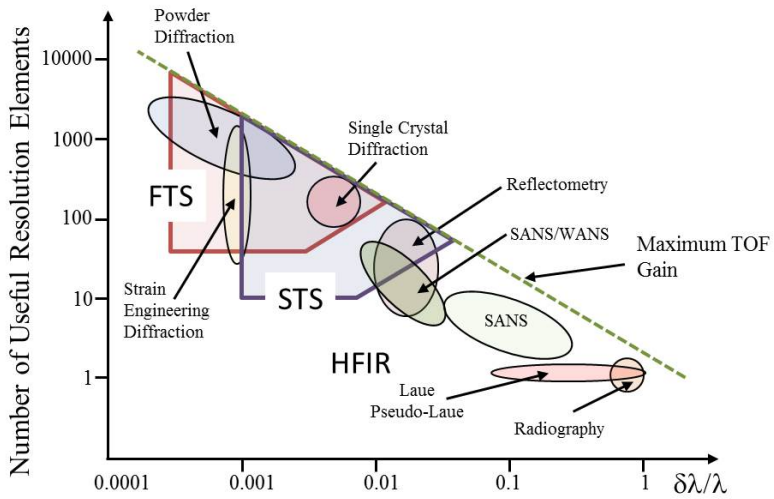

Fig. 1.10. Optimal performance map of elastic scattering instruments across the ORNL neutron sources.
Within the labeled boxes, the performance of the ORNL pulsed sources is expected to exceed that of HFIR. Outside the boxes, HFIR will obtain a desired data set more quickly.

Figure 1.11 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 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 toward 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 40× fewer 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 H2 moderator has about 5 to 7 times the peak brightness of the FTS moderator (see Figs. 1.8 [c] and 1.9). Assuming repetition rate multiplication is equally effective at both sources, these instruments will be best sited at 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 that 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.

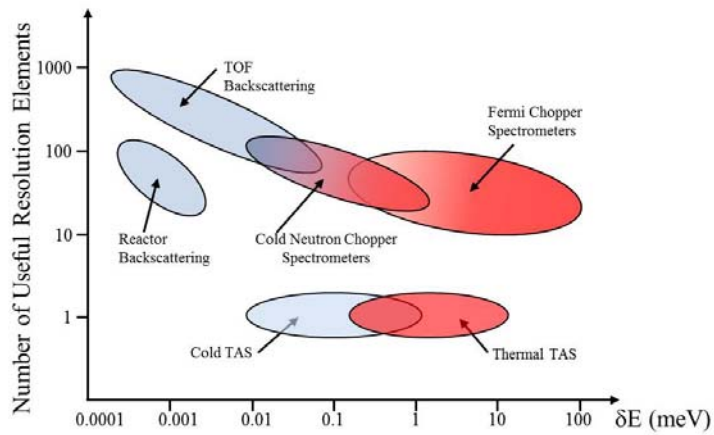

Fig. 1.11. Performance map of the inelastic spectrometers.
The colors indicate the incident neutron energy with red signifying thermal to epi-thermal neutrons and blue, cold neutrons.

1.7.4 STS Instrument Strategies

Meeting the emerging science challenges of the next decade and beyond requires new paradigms in neutron scattering instrument design and optimization. Performance gains (flux on sample, sample size, resolution, extreme environments in pressure and magnetic field) on the order of 100 or greater are required (see some of the science case discussions in the instrument concept sections). As discussed above, the current maximum projected source gains of STS relative to FTS are ~10× in peak brightness (Fig. 1.9). The remaining order of magnitude must be achieved in the instrument design or development of associated sample environments. Some of this gain can be realized by use of the newest technologies,

particularly in the area of neutron optics (which is discussed in Section 6). In general, though, STS neutron scattering instruments will inevitably tend to more specialization and less flexibility. For example, measuring smaller samples may require not only better neutron optics and beam focusing but also an increase in acceptable beam angular divergence (see Section 2.2, the CHESS concept) or development of background reduction technologies (see Section 3.3, the DyPol concept). Following are a few observations about STS instruments and their design:

- The science focus of each instrument must be well-defined because the desired performance gains are likely to push in the direction of less flexible, more specialized, and highly optimized instrument designs.

- Advances in neutron optics must be leveraged. This includes not only advanced guide technology but also development of more sophisticated optics systems such as illustrated by the HFIR IMAGINE instrument and the use of Wolter optics (Fig. 1.12).

- The smaller, high brightness moderators discussed above will enable better optimization of neutron optics systems but likely at the cost of increased mechanical complexity and possible active alignment systems. Particularly in the near moderator regions, care must be taken in the mechanical design of the target monolith to support the higher precision required. It will be important to support a close approach to the moderator of neutron optical systems, 60 cm or less.

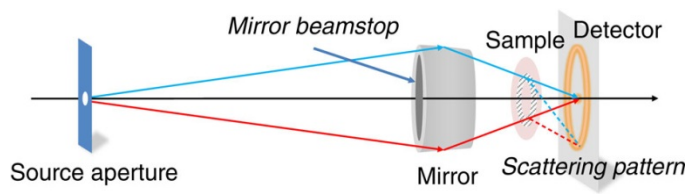

Fig. 1.12. Compact small angle neutron scattering instrument developed at MIT and tested at HFIR. [2]

- The low, 10 Hz repetition rate of STS will enable the use of much larger bandwidths per pulse, translating to the ability to simultaneously sample much larger length and/or time scales.

- Instrument concepts must mature on a time scale such that they can influence the final choices in moderator and source geometry and neutron spectral characteristics (pulse widths, brightness, and size).

- Development of neutron polarization techniques for use on TOF instruments is crucial because many of the methods commonly used on instruments at continuous sources are not directly applicable. Wide-angle polarization analyzers are particularly important because of the large solid angle detectors' coverage on most TOF spectrometers (see the science cases for CHESS and HERTZ, Sections 2.2 and 2.3, respectively).

1.7.5 References

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

[2] D. Liu, et al, Nature Commun. 4, 2555 (2013).