The Neutron Advisory Board (NAB) met in Oak Ridge 2-3 April , 2013. Present were Joel Mesot, Andrew Harrison, Douglas Tobias, Meigan Aronson (chair), Janos Kirz, Yujiro Ikeda, Bernhard Keimer, Gabriel Aeppli, and Robert McGreevy. Not attending: John Hemminger, Sharon Glotzer, and Sunil Sinha.

Charge

The NAB was charged by the NScD to provide advice and feedback on the following items:

Charge
Neutron Advisory Board
April 2-3, 2013

1. Source performance – our neutron sources must operate reliably and predictably at prescribed power levels.
2. Maximize existing instrument performance – our strategy now has a 5 year plan to build-out existing instruments, complement these instruments with sample environment and support our users with excellent scientific and technical support staff. Steps are underway to improve data collection, analysis and visualization.
3. High quality scientific output – our staffing plan, reorganization and outreach activities continue to drive improvement across all disciplines.
4. Establish the longer-term scientific strategy to meet future needs – This includes both capacity increases and new capability with priorities driven by the scientific community.

We continue to be interested in advice concerning each of these areas but it is requested that the focus for this board meeting be dedicated to priority 4 above.

The Second Target Station (STS) has been determined to be "absolutely central to U.S. world leading science." However, there remain "scientific/engineering challenges to resolve before initiating construction." It is important that we obtain your advice and *counsel on the nature of the related questions and the path for getting them resolved. This will be necessary in order to move forward with the STS.*

The capacity argument for the STS has been made by our community but we must strengthen the new capability argument for an investment on this scale. Our strategy for closing this gap must be carefully thought-out. It is anticipated that STS will support long wavelength studies, delivered by a short pulse or a long pulse. This decision is inextricably linked to instrument selection, science drivers, and the ultimate fate of HFIR.

-Kelly Beierschmitt and Thom Mason

Meeting Agenda and Outcomes

An agenda for the meeting was developed by K. Beierschmitt and M. Aronson, in consultation with the NAB. The meeting started with a welcome from Deputy Director J. Roberto (ORNL), followed by a review of the year's progress by K. Beierschmitt, and the associated discussion. As agreed, the focus of the meeting was to be the discussion of a second target station (STS) to be sited at SNS, with capabilities that would be complementary to the current first target station (FTS). The meeting began with a tutorial on the technical issues associated with the short pulse/long pulse options for the STS, presented by R. Pynn and J. Carpenter. A second presentation was made by C. Broholm that described new types of science that would be made possible by a long-wavelength, high-intensity source. Substantial discussion ensued, both during and after these presentations, which were open to the NScD staff and leadership team. The NAB subsequently went into a closed session that included R. Pynn, J. Carpenter, and C. Broholm, but no ORNL staff. After discussion, it was provisionally decided to recommend that the short-pulse option should be selected for the STS. A subcommittee (G. Aeppli (chair), R. McGreevy, Y. Ikeda, J. Carpenter, and R. Pynn) was selected to articulate the technical and scientific reasons for this recommendation. Their report comprises the first section of the appended NAB report. A second finding of the NAB was that the construction of the STS would provide the unique opportunity to optimize both the existing and planned instrument suites across all three of the neutron scattering sources at Oak Ridge, consisting of the First and Second Target Stations and the High Flux Isotope Reactor. The result was envisaged as a world-leading scientific facility with a range of capabilities and remarkable flexibility that would not be reproduced in any other neutron source, existing or planned.

The results of the NAB's discussion were reported to NScD scientific and administrative staff at the conclusion of the first day's work, and it was announced that the next morning would be spent in assembling and refining the ideas for new science at the STS that had been raised during the open discussion on the first day of the meeting. The second day started with a group discussion of these science drivers involving both the NAB, C. Broholm, R. Pynn, and J. Carpenter, as well as ~10-20 scientists from NScD and other parts of ORNL. Breakout groups consisting of both NAB members and ORNL staff were then formed in three areas: quantum condensed matter, biology and soft matter, and Chemistry/Engineering/Geosciences. Each group compiled a list of the most exciting scientific opportunities that would be made possible by the long wavelength and high intensity properties envisioned for the STS.

Recommendations:

The next six months represent a crucial period in which the scientific drivers and the source specifications for the STS must be developed in parallel. Both will be enabled by a series of scientific and technical workshops that will be held in Oak Ridge during the upcoming summer. The first part of our report is intended as a general description of major issues associated with the short pulse STS that must be addressed by the participants of the technical workshop(s), who will be charged with developing basic design parameters of the STS. The second part of our report presents an initial overview of new scientific opportunities that could be envisaged with the STS. It is expected that it will be useful in assembling a series of scientific workshops that will bring together world-leading experts from the neutron scattering community and beyond, while being inclusive to the full range of stakeholders who would benefit from the newly optimized suite of neutron scattering instrumentation that will become available at Oak Ridge. The participants of these workshops will be charged to develop an initial list of new instrumentation, and by considering the existing suite of instrumentation at FTS and HFIR, to develop a comprehensive plan for the placement of both planned and existing instruments that encompasses all three neutron sources at Oak Ridge.

Finally, the NAB recommends that a list of 4-6 initial experiments for the STS be developed over the course of the next year, with the aim of exploring new scientific opportunities that would showcase the performance and potential of the STS. We did not discuss a possible procedure by which this could occur during our meeting, but we feel that it should be developed in parallel with the organization of the scientific workshops. The scientific workshops will be very useful in bringing forward candidates for these initial experiments, as well as the teams that can most naturally develop and bring them to fruition. We suggest that the NScD and the NAB work together to commission a separate group of experts who can identify and also encourage these efforts. Ultimately, they and the NScD will be responsible for selecting the most promising ideas for further development. Funds should be made available to support the teams tasked with delivering these initial experiments, and the expert panel will be charged with providing advice and periodic review so that the initial experiments are ready to go when the STS becomes available.

The NAB would like to thank K. Beierschmitt and his staff for their hard work in preparing for this very useful and stimulating meeting, and for their hospitality throughout the visit. The participation of ORNL staff in discussions during the meeting was crucial, and we thank all involved for their many thoughtful contributions. J. Webber is especially thanked for her flawless assistance with meeting logistics. The NAB is energized by the promise of the new science that will be enabled by the STS, and very much looks forward to participating in the process that has now been set in motion to realize this much anticipated capability in Oak Ridge.

The Case for a Second Target Station at SNS that provides Long Wavelength Neutrons with a Short Pulse time structure.

The NAB was asked to consider both the scientific case as well as the technology choices for a second target station for the SNS. The panel's principal finding was that the second target station together with any upgrades of the first target station(FTS) be optimized together to assure the international pre-eminence of the entire ORNL neutron facilities. Among the technology choices, the most important is that of the proton pulse length, where either short pulses can be extracted from the compressor ring, as for the first SNS target station or for the first and second target stations of ISIS. Alternatively, long pulses can be directly extracted from the linear accelerator, as is planned for the ESS. Based on the information provided and its group discussions, the NAB concluded that the short pulse option would be most appropriate for ORNL.

Introduction

NAB convened on the first day (1 April 2013) of its meeting for general presentations as well as both closed and open sessions. Before the meeting, the panel was issued with copies of the reference documents listed in the appendix to this report. Most relevant for making the choice between long and short pulses was the joint presentation by Roger Pynn and Jack Carpenter, which revisited the relevant neutron kinematics. The afternoon discussions that followed yielded a group consensus in favor of the short pulse option, on numerous grounds that were minuted by the NAB Chairman, Meigan Aronson. On the second day of the meeting, three NAB members (McGreevy, Ikeda and Aeppli) augmented by two expert consultants (Pynn and Carpenter) to the SNS met to summarize and augment the group discussion, and assemble the present section of the report, which includes sections on the international competitive context, kinematics, engineering and risk, followed by our conclusions.

Uniqueness of ORNL Neutron Facilities: SNS in the World Context

Much of the discussion which follows is informed by the plots of peak brightness and time-averaged flux for various neutron sources world-wide, one of which is reproduced in the figure below. We are particularly grateful to Drs. Andersen, Argyriou, and Gallmeier from the ESS for providing these calculations.

ORNL already is and will be a uniquely potent center for neutron research, with

HFIR 85 MW, □$_{\mathrm{Th}}$ 1.5 x 10^{15} n/cm^{2-}s, LH_2 cold beam,

SNS FTS 1.0—> 1.4 MW, Hg target, 60 Hz, LH_2 and H_2O moderators

The plan under discussion provides a second target station for SNS,

SNS STS 300-500 kW, LH_2 moderators, with a D_2O target, 10-20 Hz operation, wavelengths ~10 Å.

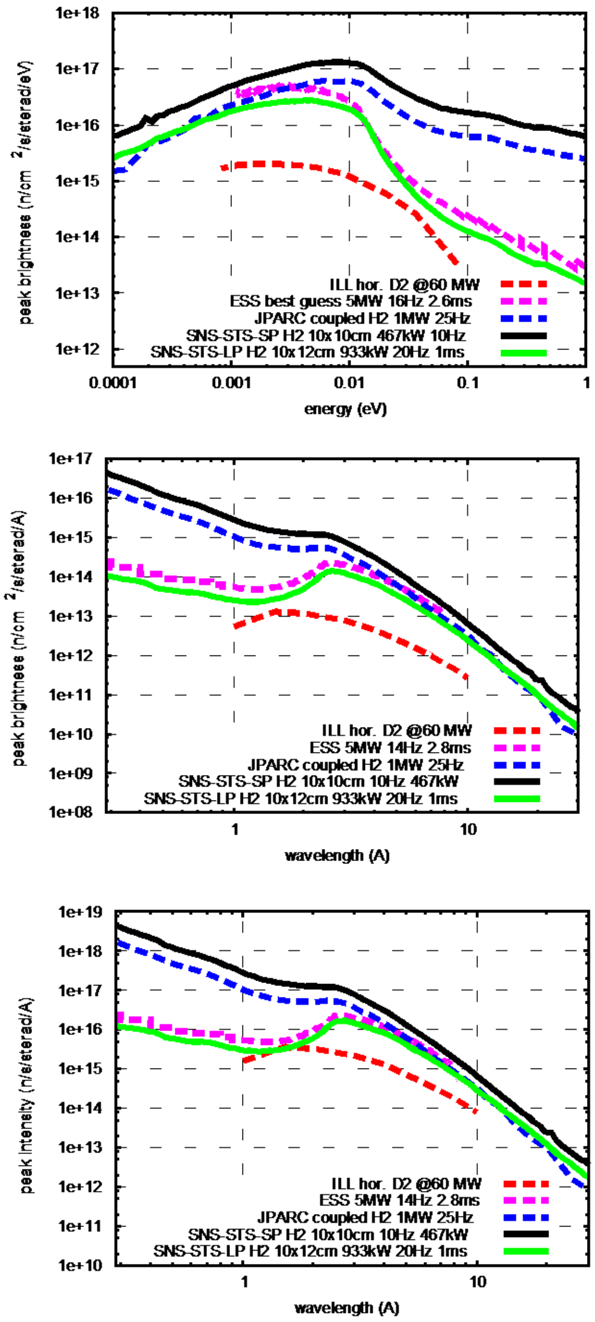
Together, these three facilities can and will support the most potent and complete range of neutron beam facilities available anywhere in the world, now and in the foreseeable future. In addition, HFIR provides world-class materials irradiation and isotope production capabilities.

For comparison, there are the following pulsed spallation sources: ISIS and ISIS TS2, JSNS, CSNS and ESS (under way), the reactor sources ILL, FRM-2, OPAL, Hanaro, JRR3, NIST, CARR, a steady spallation source SINQ, and the pulsed reactor IBR-2.

All of the existing pulsed sources maintain room temperature H_2O and most have cryogenic moderators. The HFIR and ILL give □$_{\mathrm{Th}}$ 1.5 x 10^{15} n/cm^2-s thermal neutron flux and the remaining reactors all provide fluxes 3 – 10 x 10^{14} n/cm^2-s thermal neutron flux. ILL and FRM-2 support hot sources operating at at least 2000 K and also LD_2 cold sources. The 2-MW (average power) IBR-2 pulses at 5 Hz with 250 microsecond pulses, and supports a mesitylene cryogenic moderator. SINQ gives 3 x 10^{14} n/cm^2-s and supports a LD_2 cold source. The pulsing frequencies of the pulsed sources of the recent past, of the present, and of those currently envisioned span an interesting range: 5 Hz (IBR-2), 10 Hz (TS-2, STS?), 15 Hz (ESS), 20 Hz (Lujan), 25 Hz (JSNS), 30 Hz (IPNS), 50 Hz (ISIS), 60 Hz (SNS). Among them, the experience and rationale for their targets, moderators, and instruments, might be sound bases for workshop discussions .

As envisioned, SNS STS will provide a higher cold neutron beam peak intensity than any other operating pulsed source. Its pulsing frequency, if 10 Hz, will be lower than all other long-wavelength pulsed spallation sources except ISIS TS2, and its peak cold flux will be higher than that found at any other source, existing or envisaged. The combination of these attributes will make it unique in the field and provide for instrumentation of wide ranging and unique capabilities.

ESS, a Long-Pulsed Source, will operate at 15 Hz and deliver 5 MW of proton power to the target, with 2500 microsecond-long pulses.



A comparison of the brightness and peak intensity of the proposed SNS-STS to other existing and planned sources. Figure courtesy of K. Andersen, D. Argyriou, and F. Gallmeier.

Kinematics and the Science Case

The desire to study mesoscale phenomena, that is to say structures and dynamics on length and time scales between the atomic and macroscopic, provides a clear motivation for using long wavelength neutrons. The second target station (STS) should be optimized for the production and application of such neutrons. For most applications, it will be appropriate to maximize the neutron flux by coupling the moderators at the STS. This is not to say that there is no role for decoupled cold moderators or even for thermal moderators at the STS, should a short pulse be chosen. Indeed, a careful study of these options should be part of the detailed conceptual design. We emphasize that the main focus of the STS will be to provide a maximum flux of cold neutrons with wavelengths in excess of 0.4 nm. The natural neutron pulse length provided by coupled para-hydrogen moderators is in the range of a few hundred microseconds, which provides the context for considering whether it is best to use short or long proton pulses to produce the neutrons. In the SNS context, short proton pulses would be provided by the existing compressor ring and would be ~700 ns long, more than two orders of magnitude shorter than the natural neutron pulse length, while long proton pulses would consist of an entire macro pulse of 1 msec to 2 msec duration delivered from the linac, either through part of the existing storage ring or through new beam transport lines. The committee learned that both of these accelerator options are feasible from a technical point of view and that neither is a real cost driver. Further, there seems to be little difference in the projected outage time required to install either of these options.

The use of neutron pulses of 2 ms duration leads to a natural instrument length that is longer than that required for short neutron pulses. This is because the natural wavelength resolution (i.e. the resolution obtained without the use of pulse-defining choppers) scales directly as the pulse duration and inversely as the instrument length, so that achieving good wavelength resolution naturally leads to longer instruments. To maintain a suitable dynamic wavelength range under such circumstances, it is convenient to reduce the source repetition rate. Source frequencies between 10 Hz and 20 Hz were discussed by the committee. While there was a preference for the lower end of this range, it is clear that the actual value should be determined during the conceptual design phase to maximize the scientific productivity of the facility.

The committee recognizes that the main driver for new source specifications needs to be scientific and concluded that, averaged over possible important uses of the sources, there will be little to distinguish between the science enabled by long and short proton pulses. To make this concrete, we consider a short-pulse target with a power of 46 kJ per pulse and compare this with a long-pulse target with a power of 70 kJ per pulse. We assume that we can eliminate proton pulse chopping in the former case, even though this is not yet a demonstrated option. The best we can hope for on the long-pulse target station is to design instruments whose performance scales with the average neutron flux. Thus, even if we assume that the long-pulse source operates at 20 Hz and the short-pulse version operates at 10 Hz, the long pulse source outperforms the short pulse target by a factor of 3. Conversely, for those instruments whose performance scales as the peak neutron flux, the short pulse source outperforms the long pulse by a factor of 3 since its pulse duration, even for coupled moderators, is that much shorter. While these numbers are not insignificant in the context of neutron scattering, where the average performance increase between successive generations of instruments has been estimated to be 3 – 4, averaging over a suite of instruments of various types indicates that the overall performance difference between the two types of source is unlikely to be decisive.

More decisive are the constraints and boundary conditions implied by the existing infrastructure at the SNS site, as well as cost considerations associated with the instruments. First, the site offers a limited range of flight path lengths for a new target station. At a time when the planning for the long-pulse spallation source ESS has led to several instruments that are 150 meters long, the committee learned that the longest flight path that could be envisaged at the SNS site is 120 m and that only 2 or 3 beam lines could be that long, with a large majority of beam lines being restricted to lengths shorter than 40 m. The ESS reference instrument suite comprises 15 that are longer than 50 m, with 9 of these being 150 m long. As discussed above, the natural length of a neutron instrument scales with the neutron pulse duration, so instruments designed to take advantage of short proton pulses (i.e 300 microsecond neutron pulses) are expected to fit better within the available SNS site footprint than those designed to take advantage of neutron pulses that are longer than 1 msec.

Even assuming a larger site, longer instruments carry increased costs on all fronts, from civil construction to optics and vacuum tanks.

The panel did not spend time weighing the desired repetition rate for a short pulse source. However, it notes that the WISH instrument on ISIS TS2 is already using 5 Hz for a high count rate. For this reason alone, the science will always push towards a longer frame. Anything that is optimized for 20 Hz might still be more favorable if installed on the SNS STS.

Engineering and risk

There are numerous engineering factors to consider in the choice of proton pulse length for the spallation neutron source station. They include the following:

1. Nature of the accelerator complex. A linear accelerator will suffice to produce long pulses, whereas a compressor ring is required for short pulses.
2. Target design and lifetime, which will be shorter for the stronger shockwaves associated with the higher peak brilliance of the short pulse.
3. Instrumentation, which will need to be designed differently, including chopper arrangements.

We treat each of these points in turn:

(1) is not really a deciding factor, given that the SNS already has a compressor ring, unlike the ESS, which is a green-field project. The accelerator developments required for 3 MW total power shared between FTS and STS overlap greatly, provided that STS operates in pulse stealing mode. Since this is perfectly acceptable from the neutron

instrument perspective it is the obvious choice. The accelerator development required for 3 MW total power with either LP or SP is very similar and much of this is incorporated into the planned power upgrade project (PUP) that will equip SNS to deliver 1.4 MW. The main exception is in the stripping foil in the SP case. However, this development is needed anyway if higher power is to be delivered to FTS as part of the PUP, regardless of the STS choice.

(2) One advantage of choosing the SP option in engineering/risk terms is the possibility to follow a staged approach that decreases risk considerably, but still provides significant performance gains and scientific possibilities. The STS can be built and start operation using whatever power can be provided from the existing accelerator. The existing mercury target is known to cope with the present energy per pulse with a lifetime of order six months. This is perfectly acceptable from an operational perspective. If the accelerator power were increased from 1 to 1.4 MW and ~ 300 kW were delivered to STS then performance gains of order 6 relative to the known capability of ISIS TS2 can be expected, without any degradation of the FTS performance. If the power were increased to ~ 900 kW then the gains might be of order 14. Note that there is a sub-linear scaling between accelerator power and achievable neutron count rate on any instrument. Careful consideration should therefore be given to maximizing the cost/benefit, rather than maximizing the accelerator power.

One reason for choosing a LP STS in the past would have been the uncertainty associated with the lifetime of the mercury target. However, as already noted, the present target performance is acceptable until the PUP takes place. In addition, a jet flow target is under construction that is expected to improve lifetime by an as- yet unknown amount. In addition, the He bubbler development at JPARC looks extremely promising. Although a target has yet to be run until end of life, this will be known well before any decision on STS target needs to be made. An alternative would also be to look at a solid target option for STS, e.g. Tungsten. One specific advantage of this may be that it overcomes the fire regulations that restrict the use of more than a small amount of flammable hydrogenous material in the FTS, e.g. borated wax or polyethylene, which are common neutron shielding materials. If STS is to achieve the signal to noise that will enable new science, not just the signal, it must be able to freely choose the optimum shielding materials.

For the reasons stated above, the target is no longer considered to be the limiting factor in the SP/LP decision

(3) SNS already has considerable experience with the design and construction of 60 Hz SP instruments. Experience with SP instruments at lower frequencies is available at ISIS (10 Hz) and JPARC (25 Hz). Their performance is known and can relatively reliably be scaled to higher powers. It should be possible (and has been shown at ISIS) that using the experience gained by building and commissioning the first instruments at STS using known technologies can provide significant scientific gains within a very short time of first operation. The user community will be familiar with the techniques, software will be available etc. These factors all suggest that scientific impact for the STS will be achieved much more quickly. There is no similar experience at SNS with LP instruments, which are likely to need more elaborate choppers, so a LP source would likely take longer to achieve a similar degree of impact.

Conclusions

From all standpoints – scientific case, site geometry, and engineering practicality, NAB is in favor of using the short pulse option for reference purposes during the upcoming scoping and design phases for upgrading the SNS. The panel believes that there is neither time nor resources to engage in a process to further consider this choice, especially given the compelling kinematic arguments given above as well as the need to focus the science and instrument design discussions needed to respond to the Brinkman letter. Because the Brinkman letter seeks a rough cost estimate and there are engineering choices (e.g. 10 or 20 Hz, nature of moderators and targets) even within the universe of short pulse options, we recommend that a source engineering workshop be held alongside the science workshops that must be planned to prepare the response to DOE/BES.

It is important to see the STS in the context of other international sources. The ESS is planned as a long pulse source of 5 MW. This choice has been made based on optimizing the scientific output of a facility where there is complete freedom to choose the accelerator, target and instrumentation and where there are no real space constraints. These features do not apply to the STS. At the SNS, where maximum linac power in the foreseeable future will be limited to less than 3 MW, with only a maximum of 1/3 of that directed to an STS, it is clear that a long pulse STS would inevitably underperform the ESS. On the other hand, the peak flux of a 460 kW, 10 Hz short-pulse STS could be similar to that of the ESS, depending on details of the moderator design.

The SNS has come up a long learning curve to become the world's most intense short-pulse spallation source. It has mastered the accelerator, target and instrument technology required for such sources. Were it to embark on the construction of a long-pulse target station only a part of that technology know-how would be transferable and it would find itself in the unenviable position of having to catch up with its European rival, the ESS. By building a short pulse STS, the knowledge base of the SNS can be directly transferred.

Finally, the committee points out the unique opportunity that the construction of a short-pulse STS would provide to ORNL, which would then be the site of three very different neutron sources: the FTS, HFIR and the STS. All are complementary to each other in many ways. It would be possible to site practically any neutron scattering instrument at the specific source which gives it the maximum possible performance. Treating the three sources as an ensemble to be optimized together also has the benefit of providing focus for the US$60M instrument TS1 upgrade program currently proposed to the DOE.

Towards the Development of Science Drivers and Initial Experiments for a STS and the Optimization of the Neutron Scattering Complex at Oak Ridge.

It is crucial that the best and most compelling new science be identified and then fostered in order to realize the truly new and transformative scientific capabilities of the STS. The NAB and the assembled scientific experts from ORNL worked together to compile an initial list of areas that we found especially exciting. We stress that the actual specifications of the STS are not yet determined, so we focused on experiments that would be enabled by a greatly increased flux of long wave length neutrons. These ideas are not meant to be conclusive, or to represent the entire range of new science that may be possible. It is our suggestion that these ideas should serve as initial input for the scientific workshops, where they will be refined and expanded by the participants.

Our suggestions are organized within familiar disciplinary bounds, but we note that there are several different crosscutting themes.

1. Experiments where the neutron beam or an external radiation source induces unusual excited or transient states, where time resolved studies can be used to study the approach to the normal ground state.
2. An expanded use of imaging, over a broader range of length scales.
3. The ability to probe dynamics in systems where a hierarchy of length and time scales are needed to describe the functionality.
4. New opportunities to carry out neutron studies of matter in extreme conditions, such as high magnetic fields, pressure or temperatures, as well as *in situ* for both devices and biological systems.

1.Quantum condensed matter

A.Magnetic mesostructures Mesoscopic magnetic structures such as skyrmion or vortex lattices have recently attracted considerable attention in quantum condensed matter physics. These structures can be imaged by magnetic neutron scattering with cold neutrons. Static structures are also accessible to alternative probes such as Lorenz microscopy in some cases (although such experiments require special sample preparation), but the corresponding collective magnetic excitations are typically in the sub-meV regime, and are not accessible to complementary techniques such as electron or x-ray scattering. Neutron scattering from the excitation sidebands generated by magnetic mesostructures require the greatly enhanced energy and momentum resolution offered by the STS. Experiments at the STS will also provide access to the nonequilibrium dynamics of such structures under current flow.

Magnetic neutron diffraction and off-specular reflectometry at the STS will have sufficient intensity to resolve in-plane magnetic superstructures in thin films and devices, which today can only be done with neutrons or soft x-rays in some special cases. This will also enable in-situ measurements of magnetic structures in spintronic devices under operating conditions, which will be important for device applications.

B.Quantum critical points At the zero temperature phase transition between different states of matter there can exist a quantum critical state with unique and universal properties. Generically these states are characterized by long length and time scales and by novel emergent properties that may be associated in some cases with fractionalized quasi-particles. Many anomalous phases of materials that can be appreciated even at room temperature are now thought to be a consequence of such underlying quantum critical phases.

Probing the essentially dynamic quantum critical phases is of the utmost importance and requires (1) the ability to realize the quantum critical state which means ultra low temperature capabilities often in combination with high pressure and high magnetic fields (2) inelastic neutron scattering capabilities in the corresponding energy range which extends from 1 μeV to 10 meV. In general the full range of wave vector transfers is needed, with emphasis on the <3 A^{-1} range. The low Q range is often of great importance even though there may be little intensity there, because it relates to the hydrodynamic description of the critical state. The ultimate sensitivity is required to make these experiments possible. The low-temperature, low-excitation-energy experiments will be very hard to perform with x-rays.

There are cases in which the critical or spin liquid state carries more complexity within it that cannot be appreciated through experiments under equilibrium conditions. To appreciate the nature and range of topological quantum order or long range entanglement at the critical point, it may be necessary to probe non-equilibrium properties in a pulse probe mode. Observing the process by which the system returns to the equilibrium state from a perturbed state will hold valuable information that can distinguish different quantum critical universality classes.

C.Measurements in High Magnetic fields We can anticipate that the state of the art of magnetic field capabilities will have improved considerably by the time STS is built. In particular, we believe the following will be possible:

- pulsed split coil: 50T (~5 mins between pulses)
- pulsed solenoid: 70T (~10 mins between pulses)
- high-Tc tape DC magnet: 25 T portable; 35 T fixed

In all cases, the STS low rep rate gives larger bandwidth which is advantageous when there are restrictions on scattering angle. For the pulsed magnets, the high peak intensity is particularly advantageous. It is most likely that pulsed magnets will be used primarily for diffraction. For inelastic scattering the energy scale is well matched to a long-wavelength target station or a cold source at a reactor.

The combination of high fields and variable temperature enables exploration of new regions of phase diagrams in many materials showing magnetic order. This will be useful both at diffraction instruments and SANS instruments. Examples of new science that can be accessed include HT phase diagrams in multiferroics, helical magnets, and unconventional superconductors. Detailed investigations of field induced spin-density wave states (e.g. organic charge transfer salts) and other exotic states will become possible. When high magnetic fields are combined with low T and high P one will be able to explore the physics of quantum critical points in great detail in the combined phase space. The time structure of pulsed fields will permit kinetic experiments looking at time dependencies of both magnetic structures and materials structures that are influenced by magnetic fields. Examples might include relaxation of spin glasses or antiferromagnets which have been excited into a ferromagnetic state. With steady state fields, one can use inelastic neutron scattering to explore excitations in exotic field-induced states.

II.Chemistry, Engineering and Geo-sciences

Overall Objectives:

To follow hierarchical growth processes, chemical transformations and defects and distortions in materials from the atomic to the mesoscale in real time and in-situ. This can be achieved through direct imaging, scattering, and spectroscopy.

The range of relevant length scales requires a complementary suite of scattering instruments at HIFR, FST and STS, and will be essential for a wide range of user communities, from academia to (US) industry.

A.Imaging Direct neutron imaging has seen impressive developments in the past 10 years. This includes on one hand Bragg edge and phase contrast, and on the other polarization contrast providing enhanced contrast methods. Such methods will be particularly powerful at STS. Fast imaging capability will be essential for 3D Tomography.

- Flow of fluids through porous media such as electrolytes through membranes in fuel cells, batteries (imaging H, Li with 1 micron resolution), fuel injectors.
- Fluid flow in sub-surface environment: relevant for example for ground water management, waste processing, fracking, carbon sequestration. etc…
- Processing of biomass in reaction vessels, characterization of morphological changes over broad q-range, neutrons offer enhanced contrast between components because of different H contents.

B.Spectroscopy Optimization of hot neutron source on FTS for molecular spectroscopy up to 1 eV in environments opaque to IR and Raman. Potentially huge community, since much research on chemical catalysis would benefit from such capability.

C***.Diffraction*** Solvo-thermal chemistry: In-situ observation of chemical processes from nucleation to crystallization. Issues: intensity due to dilute systems; hydrogen location is in majority of the cases essential; High-temperature, high-pressure environments. Relevant for geo-sciences too: mineral formation. Generally requires extreme conditions (high-P, high T).

Extreme conditions (high-P, high T) may also be exploited in the chemical synthesis of metastable structures, and the exploration of (P,T) phase diagrams that might point the way to new, metastable functional materials (diamond, for example, is a metastable substance at moderate values of P and T).

Understanding the impact of processing conditions on the properties and performance (mechanical, electrical, thermal) of (engineering) material (including metals, ceramics, composites). In-situ capabilities will be essential (heat treatment, stress, …)

High resolution diffraction studies to underpin the search for novel materials with enhanced performance – complementing the trend to explore yet more complex architectures (metal-organic framework materials (MOFs), hierarchical structures…), and in the case of porous materials also to explore the structure and processes of sequestered molecules. The combination of a wide range of Q, with high resolution and flux provided by optimized diffractometer on STS will be transformative.

A key challenge in 'materials by design' is a deeper understanding of self-assembly and the possibility of self-repair in soft materials. New insights will be provided through the resolution of structural and dynamic details of solvent-mediated. Enhanced capability for reflectometry and grazing-incidence scattering (wider range of Q and enhanced flux – and thus faster time-resolution at the STS, will enable a new generation of developments in designed, self-assembled materials.

The interactions of reactants with catalytic surfaces, potentially in combination with temperature or photon enhancements hold keys to next generation advances in heterogeneous catalysis and surface chemistry. The wavelengths and energy ranges accessible at the STS are well matched for investigating the surface-mediated interactions driving new controls in catalysis.

III.**Biology and Soft Matter:**

A.Seeing hydrogen atoms and ions in membrane proteins. Membrane proteins, which comprise roughly 30% of the genome, are involved in crucial physiological processes such as signaling, energy production, and the transport of chemicals and ions in and out of cells and between cellular compartments. An important class of membrane proteins is the voltage-sensitive ion channels that are responsible for electrical signal transmission along cell membranes. Ion permeation pathways are lined with ionizable sidechains that participate in the ion conduction mechanism, but their protonation states are difficult to ascertain definitively by other techniques. Although membrane proteins are notoriously difficult to crystallize, roughly 300 unique membranes have been crystallized and have had their structures determined by x-ray crystallography to date. The resolution of membrane protein structures is typically lower than that of soluble proteins and, hence, hydrogen atoms are not resolved, and it can be difficult to establish the identity of similarly sized species, such as Na+ and K+ ions. With isotopic substitution, neutrons are capable of differentiating between solvent and ions (e.g., metal cations: Na+, K+) within the channels, and establishing the protonation states of ionizable residues. Present neutron protein crystallography instruments require large crystals (e.g., ~1 mm^3 on Mandi), which is prohibitive for membrane proteins. The increased flux at long wavelengths on the STS would enable smaller crystals, ~0.01 mm3, to be studied. In addition to making structure determination of membranes possible, this opens up the possibility of doing freeze trap studies of kinetic intermediates in enzymatic reactions for which proton transfers between substrate and protein and/or water play a key role but are not resolved by x-ray crystallography. The mechanistic insight provided by neutron protein crystallography could have a major impact on drug development.

B.Time-resolved studies of protein aggregation. Protein aggregation, i.e., the formation of insoluble protein aggregates, is implicated in a number of diseases (e.g., Alzheimer’s, Parkinson’s, and Huntington’s diseases), and limits the efficacy of protein-based pharmaceuticals (e.g., monoclonal antibodies). The mechanism of protein aggregation is poorly understood. SANS has proven to be a useful technique for structural studies of aggregated proteins, but the limited angular scattering range covered by current instruments prohibits time-resolved studies. A broad Q-bandwidth, short-pulse STS opens the door for SANS measurements in which the utilization of the time structure for post-measurement parsing into bins that optimize both time resolution and signal-to-noise (e.g., EQ-SANS). In addition to protein aggregation, this capability introduces time as a variable in studies of the formation of large, multi-component protein complexes.

C.Polarized Neutron Analysis. The increase in the long wavelength neutron flux at SNS's proposed 2nd target station will enable the practical development of a polarized SANS capability, a technique that has yet to be routinely implemented in biology. Using polarization techniques allows the study of biological systems over an extended q-range suppressing the incoherent background from hydrogen without need for extensive deuterium labeling.

D.Pump-probe studies of biological molecules. Biological processes enable life through complex processes that span a wide range of time and length scales. Protein complexes function through interaction and docking and conformational changes on the time scales of hundreds of nanoseconds to microseconds, but cellular processes that build on these fundamental steps span into the time scale of minutes. One example is the rearrangement of intracellular membranes in cyanobacteria in response to changes in light intensity. One challenge in studying ensembles of dynamic systems is to overcome the averaging over a population, this can be overcome through pump-probe studies, i.e. by stimulating the large majority of an ensemble into an excited state by changes in chemical potentials, pH, light, microwaves, electric fields and measuring the response over microseconds to minutes, and atomic to micrometer length scales.

E.Characterization of morphological changes during the processing of complex materials. E.g., biomass degradation, over a broad Q-range via SANS. Currently, can only look at narrow Q-range. Neutrons penetrate into the reaction vessel. Individual components can be followed using H/D contrast.

F.Membranes and membrane proteins in their natural state. Currently, limited Q-range prohibits time-resolved reflectometry. STS will enable in-plane structure and organization of individual components to be determined via grazing-incidence diffraction.

Additional notes:

Through the improved flux and broader bandwidth provided by the STS that will both expand the range of systems and sample concentrations that can be studied, as well as greatly improve the efficiency of the data collection, the breadth of structural biology questions that can be addressed will increase. Kinetic processes, such as the activation of the Protein Kinase A complex in response to an signal received by a cell, can be investigated *in situ*.

Drug delivery is as important to an effective pharmaceutical therapy as the specific chemistry of the drug. The formulation, encapsulation and specific release mechanisms are all of vital importance for achieving optimal performance, yet the interactions between the drug and carrier during the self-assembly process of encapsulation and subsequent release remains unknown. The high flux and wide wavelength bandwidth afforded by the STS would enable *in situ* studies of the self-assembly during formulation and stimulated release processes with sub-second resolution, which is currently not possible at existing neutron scattering facilities.

The improved flux and broader bandwidth provided by the STS will provide a new set of neutron scattering characterization tools uniquely suited to the investigation of meso-scale systems across length scales and time scales that are currently not attainable by available technologies. The realization of these tools will be felt in many areas including high performance materials and systems for energy/ automotive/ aerospace applications, biomedical, etc.

With an order of magnitude increase in brightness at the STS, the sample area can be reduced 10X, or alternatively new parametric studies with several samples may become feasible. One potential impact would be to produce and characterize new patterned substrates optimized for freely suspended films as functional materials in an aqueous environment. One example would be a new platform for lipid bilayers with functional transmembrane proteins for use as sensors or in biological studies.

The extremely weak scattering resulted from the use of zero average contrast and small sample aperture requires a significant amount of time for obtaining a reasonable count statistics at low Q domain where a large structure (i.e. 300 nm) is probed. It is estimated that beam time allocations of at least ten days are needed for PEO/silica system at the present facilities. The STS is expected to reduce significantly the counting time. Also the studies will benefit from the high Q resolution (dQ/Q) to investigate the interactions between the nanoparticles.

A quantitative understanding of perturbations on polymer structure due to geometric constraints remains a challenge. The current knowledge on this topic is primarily from simulation. The time resolved neutron scattering experiments are limited severely by the insufficient neutron flux of the presently available facilities. The 10x higher flux of the second target and a wider simultaneous Q range in a single measurement will enable such kinetics studies.