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Professor Collin Broholm

June 18, 2004

Dr., Dir. Thom Mason,
Spallation Neutron Source
701 Scarboro Road
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Email: masont@sns.gov

Dear Thom,

Please receive the report from the April 2004 meeting of the Experimental Facilities Advisory Committee. We appreciate all your help and hospitality during the meeting.

EFAC had a very positive impression of the progress being made across the Division and there are no major concerns to report. Target recommendations relate to manufacturing and plans for tests and operations. The integrated reflector plug will continue to require close attention to ensure a positive outcome. On the instrumentation side, funding of the SING project is great news. We are also pleased to see growing activity in the important area of data analysis software development. High on the list of items to consider for contingency funding should be more detectors for POWGEN3 and earlier acquisition of sample environment systems. Finally, you will note that we modified our recommendation on the USANS LOI since the closeout session owing to the positive result of peer reviewing.

Please don't hesitate to contact me or others on EFAC if clarification is needed.

Sincerely,

Collin Broholm

EFAC Report for April 2004

A meeting of the Experimental Facilities Advisory Committee (EFAC) of the Spallation Neutron Source was held from April 14 to April 16, 2004 at the SNS headquarters in Oak Ridge, Tennessee. EFAC members present at the meeting were G. Bauer, M. Bourke, C. Broholm, T. Broome, C. Carlile, J. Copley, R. Eccleston, J. Jorgensen, K. Kakurai, D. Myles, G. Russell, and D. Tobias. N. Balsara, F. Mezei and S. Nagler were absent. Bruce Gaulin, James Richardson, and Noboru Watanabe participated as observers.

1. Executive Summary

Excellent progress is evident throughout the SNS project and there are no major concerns to report. The present section contains a brief summary of findings and recommendations most of which are detailed in subsequent sections.

An important positive development since the last EFAC meeting is approval of DoE-BES funding for a next generation of SNS neutron scattering instruments. The SING project provides construction funding for five instruments that have all previously been approved by EFAC. This approximately $70M investment will have a substantial positive impact on the scientific output from SNS over the next two decades.

The progress and planning of the target system installation phase is outstanding, and EFAC would like to congratulate the whole team. The success of the installation so far gives confidence in the ability of the team to meet the challenges of the critical tasks to come.

The target module manufacturing contract was awarded in March and EFAC is confident that this procurement will yield an adequate target for early operations. Nonetheless, analysis and test experiments must continue to ensure that improvements in target durability keep up with the increased proton beam power through commissioning.

The integrated reflector plug is also in manufacture. EFAC remains concerned about the complexity of the design and the potential schedule risk from manufacturing problems. Fortunately SNS is paying very close attention to the manufacturing process and together with the vendor some important simplifications have already been made.

Apart from manufacturing and installation, much activity is presently devoted to planning for target system tests and operations as is appropriate for a complex and tightly regulated facility. This important work is being carried out in a systematic and professional manner and EFAC has confidence in positive results.

EFAC received an update on progress with the POWGEN3 powder diffractometer. This is now a mature project well on the way to becoming a formidable tool for rapid and complete atomic scale structure determination across the materials sciences. We were pleased to hear that current plans call for completion of installation in September 2007. However, it is important that this installation includes a substantial fraction of the 42 m^2 detector bank so the instrument can demonstrate the third generation concept during early operations.

EFAC received a second and updated Letter of Intent (LOI) from an IDT interested in developing a time of flight Ultra-Small Angle Neutron Scattering (USANS) Instrument. The LOI describes an instrument that bridges the gap between conventional SANS and light scattering and which is well suited to be the upstream partner of a shared beam line. Following the meeting, EFAC solicited referee reports from an international group of SANS and USANS experts to better evaluate the scientific potential for this technique. The responses received indicate considerable scientific interest in probing length scales from 0.01 μm to 100 μm through neutron scattering. EFAC therefore recommends acceptance of the LOI. In developing a full proposal, the IDT and SNS need to identify an existing or future partner instrument to share a beam line with TOF-USANS.

Apart from completing instrumentation hardware, much work remains to develop software capable of analyzing the massive neutron scattering data sets that will soon start to emanate from SNS instrumentation at an unprecedented rate. Existing programs form a complex and inadequate patchwork that would be a bottleneck for scientific output and for attracting new users. Fortunately, there is considerable interest within the neutron scattering community in rectifying this situation and this presents a unique opportunity for SNS. To ensure a coherent and extendible software suite that will work when needed at the SNS, the facility must however, play a leading role in coordinating activities in this area. The recent software development workshop, a white-paper describing SNS needs for analysis software, and the arrival of SNS software team leader Steve Miller, are all signs of growing attention to this important area.

As operations near EFAC looks forward to more attention being devoted to development of the scientific program for SNS. The recent hire of two condensed matter physicists to start a theoretical group is a welcome and important step forward as are the cross appointments of SNS instrument scientists with relevant ORNL scientific divisions. As instruments move into the detailed engineering design phase the corresponding IDTs and IATs are an additional important resource that SNS can draw on to develop plans for early spectacular experiments that will showcase the capabilities of the new facility.

2. Target System

2.1 The Target Module

The contract for target manufacturing has been awarded in March with three (minor) modifications relative to the earlier design:

- contrary to the original planning the target can presently not be kolsterized as a whole after welding, because of constraints in the process equipment;
- the transition piece between the target vessel and the mercury pipes has been modified and is now one single piece providing the transition for all mercury feed and return lines;
- a stiffening baffle plate has been added along the symmetry plane of the target vessel to shift the natural frequency of dilatational oscillations from 70 Hz to 280 Hz in order to eliminate the risk of resonant excitations by the 60 Hz pulse.

2.1 Comment: The Committee is confident that a suitable solution for the kolsterizing issue will be found and has no worries in this respect.

The new design of the transition piece is clearly an improvement, making assembly easier, stiffening the whole structure and reducing the risk of a mercury leak to the target vault. With respect to the baffle plate down the center of the target right where the beam intensity is at its maximum, the Committee does have some concerns, although the designers claim that it has minimal effect on the flow and that stresses and temperatures from direct heat deposition are acceptable: In full power operation this plate will be subject to high radiation damage, rapid thermal cycling, cavitation load, high radiation damage and, since it ties the upper and lower wall together, added mechanical stress from the pressure pulses (fatigue).

2.2 Recommendation: The Committee was under the impression that detailed studies of these combined loads have yet to be performed and recommends that they be done in full thoroughness.

These concerns are clearly not an issue for the first target, which will not see full beam intensity for any extended period of time, but confidence needs to be built for the longterm operational safety. A piece of metal breaking away from the baffle plate might cause serious damage in the mercury loop.

The Committee also noted that, despite some difficulties on the part of the European partners, the international collaboration on highpower targets continues to produce valuable data that may ultimately lead to a quantitative understanding of the pressure wave generated cavitation erosion. Again, the new work, albeit not necessarily fully representative of what is going on in a beam-induced pressure wave, seems to underpin the importance of finding a pressure wave mitigation technique. Observation of the surface acceleration on the liquid metal container of the Magnetic IMpact Testing Machine (MIMTM) experiment with high time resolution seems to give important clues on the phenomena going on inside the container.

2.3 Recommendation: The Committee strongly supports the use of detailed flow diagnostics also in the next experiments at WNR to examine how the results depend on whether the pressure is generated in the volume or through the surface of the liquid metal.

2.2 The Inner Reflector Plug

The Committee notes with satisfaction that the Project Team devotes maximum care to the manufacturing of this crucial item. Intense and frequent interactions with the manufacturers have lead to significant simplifications of the design, eliminating some of the most critical welds and most difficult manufacturing procedures.

2.4 Comment: The Committee supports every one of the changes agreed upon with the manufacturers and welcomes the measures being taken to monitor all aspects of the manufacturing process. The Committee also concurs with the decisions, to combine several of the leak tests during manufacturing, not to fabricate a prototype of the split plate, and to defer pressure testing of the split plate until the pipes have been added.

There remains some concern that the screws used to hold the two halves of the split plate together might be subject to Irradiation Assisted Stress Corrosion Cracking (IASCC) mediated by stagnant water that might penetrate into the gap between the plates. This, however, cannot be tested prior to the use of the reflector in its radiation environment.

2.5 Comment: Given the level of detail in the discussions with the manufacturers and the decisions already taken, the Committee cannot find anything extra to suggest at the present stage.

Despite the welcome – and necessary- design simplifications, the inner reflector plug remains one of the most complex items of Target Systems and continues to carry a considerable risk of delaying the Project, if something goes seriously wrong in the late stages of the assembly process.

2.6 Comment: Although the Committee acknowledges that a simpler backup reflector plug could not be afforded, given the cost of the integrated one, we remain concerned about the increase in risk introduced by this decision.

2.3 Neutronics

The Committee notes the careful sensitivity study of the SNS performance with D_2O and H_2O reflector cooling for the integrated reflector and supports the use of H_2O cooling during the startup phase of the SNS. It is interesting that the neutronic performance of the coupled moderators is essentially independent of the coolant type, and that differences exist in the RMS deviation in all moderators when D_2O is replaced by H_2O. The explanation of differences in the RMS being due to the differences in moderator slowing down power is quite reasonable. The 15% loss in intensity for the decoupled moderators when the D_2O cooling is replaced by H_2O cooling is an acceptable compromise for the SNS during the startup phase.

2.7 Recommendation: The loss in intensity from light water should be re-considered when the SNS reaches full-power operation, because a 15% neutronic penalty for the decoupled moderators that service 2/3 of the SNS instruments is significant, and the investment to return to D_2O might very well be worth the cost.

2.8 Comment: The Committee supports the removal of the cadmium decoupler in the outer reflector. The cost savings of ~$400,000 to the project is significant – good job in paying attention to neutronic details.

2.9 Comment: The Committee fully supports the choice of methods proposed for neutronic measurements to support CD-4. Having a calibrated detector for measuring absolute neutron beam intensities will be an important tool for the SNS to have. The Committee was reassured that proton beam intensity measurements can be made with the required accuracy.

2.10 Recommendation: The Committee fully supports and encourages any effort to carry out neutron scattering measurements at the time when the CD-4 measurements are performed.

2.4 Integrated System Testing

The Committee is very impressed by the detailed work going on to plan and prepare the testing program. We also note and strongly support the principle that quantitative success criteria will be defined for each system test.

The Committee is still concerned that the list of tests being developed represents more work than may be possible in the time available. This could lead to 'shortcuts' being taken in some areas in particular, in the test program for component handling in the hot cell. The Committee is concerned that merely checking for visibility and accessibility of all connections and joints that need to be opened in case of a component replacement may not be sufficient to ensure that components can actually be replace with the remote handling equipment available. In particular, not fully demonstrating remote replacement of components with a known risk of failure (such as the mercury pump and heat exchanger) may turn into a burden on source availability once replacement becomes necessary. A major issue in these cases is remote leak testing.

The Committee strongly recommends that the tests are carefully prioritized from the outset into:

- Those which are mandatory

- Those which are highly desirable
- Those which could be eliminated with acceptable risk to operations

There is a danger in developing an all encompassing list that completion of all items will be insisted on before approval to operate is granted. Really vital tests should not be compromised by spending time on less critical ones.

It is vital that there is contingency in the testing schedule to allow for remedial work if some of the testing reveals the need for modifications.

2.11 Recommendation: Integrated target system tests should be carefully prioritized to identify those which are mandatory and ensure that there is adequate time and resources to complete and respond to those.

2.5 Planning for Operations

Production of the quantity (and diversity) of the documentation required by the regulators presents a formidable challenge and will require a great deal of effort. It is crucial that this work is adequately resourced. It is also important to ensure that as staff move off the project their knowledge (which is required for the documentation) is captured. There will inevitably be conflicts between providing resources for commissioning and testing and providing input for the documentation. The latter must be given sufficient priority.

2.12 Comment: The Committee fully supports planning for operations and the detailed approach being taken given the regulatory burden which applies to the project. The Committee considered the planning to be sound with all obvious problems being covered.

2.6 Remote handling and Target Change

It will be important to include time (contingency) for recovery when the operations do not turn out quite as planned. It is worth considering scheduling remote handling operations at 8 hours per day, leaving natural contingency. (At ISIS work is planned to give daily objectives and the team may sometimes have to work overtime to achieve these. If the work scheduled takes less than time scheduled the work is often stopped to ensure the teams get adequate rest as remote handling is both physically and mentally taxing.)

Planning of the target change has, so far, been given the most attention. Several joints have to be broken and remade and the time for leak testing appears very short. This should be reconsidered. However, even if the total time taken for a target vessel change were significantly longer than currently estimated that would not present a substantial operational issue.

The same level of detail will also be needed for planning other active handling operations.

2.13 Comment: The Committee considers the level of detail in the planning of remote handling operations to be both impressive and essential.

2.7 Interfaces with ASD

2.14 Comment: The Committee considers that the crucial interface to the Accelerator Systems Division is now being very well managed and covers all that is required with excellent co-operation between the teams.

3 Review of Ongoing Instrumentation Development Projects

3.1 SNS Powder Diffractometer – POWGEN3

The committee was very impressed with the progress on POWGEN3. This diffractometer will clearly achieve the SNS goal of being the best in its class when it is completed according to design specs. It will have high enough resolution to complete with the world's best high resolution instruments for most problems (where particle size often imposes a limit on the resolution that is useful). At the same time, it will have a high enough data rate to compete with the world's fastest powder diffractometers for many problems. It appears that adequate attention is being given to detector design to achieve the desired performance by the time detector procurement is possible. The committee was pleased to learn that the installation schedule has been moved up so that installation will be complete in late 2007. This instrument will serve a large community; it is important to have it operational as quickly as possible. The constraints on the budget for POWGEN3 continue to pose a significant concern. No actual budget numbers were given to the committee, but it was stated that only about 5 m^2 of the 42 m^2 detector bank would be populated at startup, with the hope that the remaining detectors would be installed later using operating funds. A detector area this small at startup clearly means that the instrument will be operating at only about 10% of its capacity. Depending on how the limited number of detectors are distributed, it may not be possible to operate the instrument in its intended mode where counts from all detectors are combined into a single histogram with extended d-spacing coverage. This would mean that the instrument would not achieve the "3rd generation" characteristics that make it unique.

3.1 Recommendation: We urge the Project to do everything possible to bring POWGEN3 on line with a larger detector area that will make it possible for the instrument to quickly demonstrate the power of this new design concept.
3.2 Recommendation: In the near future, attention should be given to the data focusing and analysis methods needed to fully exploit this instrument.

3.2 The SING Project

We were impressed that $64M to $75M funding for this important extension program to the SNS instrument suite has been so quickly agreed. We were pleased to hear the commitment of DOE program managers. SING is fortunate to have secured the services of John Haines as the Project Leader and we feel reassured that the program will be well-managed. It is clear that there is already a team-spirit emerging – a project within a project, but we also note that it is well integrated into the bigger project itself.

3.3 Comment: SING will have a dramatic positive impact on the scientific output from SNS.
3.4 Comment: At their autumn 2004 meeting, EFAC would like to review individual SING instruments, perhaps starting with SNAP, SEQUOIA, and HYSPEC

4. Cross Cutting Neutron Scattering Instrumentation Issues

4.1 Stray Field Limits

SNS should be commended for their early and comprehensive consideration of the potential interferences associated with magnetic fields. However, extreme sample environments are expected to be fertile ground for new science. Amongst these are high magnetic field experiments, which are likely to form an important part of the scientific program at SNS. It is therefore important that the limits on stray fields do not impede use of conventional and advanced high magnetic field systems at the SNS.

By far the most sensitive experiments are scattering instruments that rely on neutron spin echo and the fundamental physics beam line. While ^{3}He spin polarizers also require a controlled field environment, we estimate that interference only occurs when the high magnetic field is required on the instrument that is using the polarizers. Therefore interference between instruments is not expected to be an issue for this application. The experiments requiring ultra low fields and field gradients must be accommodated as well but as they are likely to be the exception rather than the rule it is appropriate to define localized field exclusion zones around those particular experiments rather than a global policy.

To anticipate future instrumentation requiring low stray fields, it would be prudent as part of an overall ALARA policy for stray magnetic fields to include large diameter field compensation coils around the sample location on instruments where high magnetic fields will be used. In addition, to anticipate these high field experiments it is important that instruments where high field experiments may occur contain only magnetically inert materials close to the sample position.

4.1 Recommendation: Limits on stray fields should *not* preclude the use of conventional and advanced high field systems at the SNS including uncompensated superconducting magnets.
4.2 Recommendation: Field exclusion zones should be defined around instruments that are particularly sensitive to stray fields.
4.3 Recommendation: Implement a magnetic stray field ALARA policy that encourages mitigating techniques such as field compensation coils around instruments that may employ high magnetic fields.

4.2 Sample Environments

EFAC was pleased to receive a purchasing list for sample environment systems during the meeting. The list contains $3.5 M for standard SE equipment and $3.5 M for specialized equipment. It is an appropriate complement of equipment to support early operations on a growing suite of instruments. Various mostly external funding sources are now being pursued for the specialized equipment with long lead times. The plan is to purchase the more standard sample environment systems from operation funds. EFAC is concerned that the lead time from issuing a purchase order to having functional equipment available for users may be longer than expected even for so-called standard equipment so that availability of sample environment systems could become a bottleneck for science. In working to deal with this challenge IDTs and IATs should be useful partners.

4.4 Recommendation: A high level of priority must be assigned to building the inventory of sample environment systems as early as possible. Internal as well as external funding sources should be aggressively pursued to ensure that sample environment systems do not become a limiting factor.

4.3 HYSPEC Placement

HYSPEC is currently the only spectrometer planned for the SNS which will offer a polarization analysis option. Moreover the use of Bragg optics to focus the incident beam should make HYSPEC complementary to the other chopper spectrometers and particularly well suited for measurements on small single crystals. The mobile secondary flight path vessel, however, means that the instrument has a large footprint, which encroaches onto adjacent beam-lines. From the information available to us it would appear to be very difficult to accommodate an instrument on beamline 15 while HYSPEC remains in its current location and configuration on beamline 14B. We are also concerned about the practicality of locating HYSPEC, an instrument on which a high proportion of experiments will require the use of a superconducting magnet, in such close proximity to NSE and the fundamental physics beam line, which are both affected by very low stray fields.

4.5 Recommendation: The HYSPEC IDT and SNS should work together to refine the instrument configuration and location so as to ensure that there is sufficient space for an instrument to be located on B15, without significantly degrading the performance of HYSPEC.
4.6 Recommendation: Conditions should be devised that enable simultaneous execution of a high field experiment with a conventional superconducting magnet on HYSPEC with demanding experiments on the neutron spin echo machine and on the fundamental physics beam line.

4.4 Data Acquisition and Analysis Software Development

Rick Riedel described and demonstrated the front end data acquisition system for SNS instruments. It was apparent that this part of the project is making excellent progress and will be ready to serve even the most demanding applications. Work remains to define the user interface for the data acquisition system. This is a considerable and a very different challenge that will require strong interactions with users, instrument scientists, and the data analysis software development team.

Plans for higher level data analysis software remain in a state of flux. During the meeting EFAC was presented with a draft functional requirement document developed by the SNS following the NESSI workshop. While somewhat uneven in the level of detail (possibly due to the draft status), the document sets exciting objectives for future developments. Because of the rapidly expanding capabilities of neutron instrumentation as well as the explosive growth in computing power there is a unique opportunity for dramatic progress in software for neutron scattering. There is a real potential to revolutionize the execution of and the output from neutron science. This should be a community-wide activity with assured broad access to the resulting infrastructure. In the earliest stages, the project must be led by the SNS, and a pre-requisite is that the resulting software be able to serve the needs of Best-in-Class instrumentation at the SNS. However in the long run, greatest value will be derived from a "group effort" producing a result that is not overly SNS/ORNL centric, and that therefore can be used throughout the neutron scattering community. The challenge for the SNS is to leverage this community interest towards development of innovative software that can be deployed in time for user operations. Based on past experiences there may only be a rather limited window of opportunity to get this right. Once different non-compatible solutions proliferate and gain acceptance amongst users, it will be difficult and costly to instill a coherent approach.

It is thus imperative that the SNS project quickly resolve the issues surrounding the respective roles of: (1) the SNS project, (2) the DANSE project – centered at Cal Tech, but including university and laboratory PI's throughout the US, (3) other US neutron facilities, and (4) the international neutron community. A sizable fraction of the university-based neutron community is poised to address fundamental issues of data analysis specific to various TOF neutron scattering instruments, in support of the DANSE design project. It is in the interest of SNS and DOE to coordinate this effort for maximum impact.

Another absolutely critical component of the software development is the integration of analysis and data acquisition for intelligent control of experiments. This issue was discussed at some length in the October 2003 EFAC report. This will presumably be addressed at some level by the data acquisition system developers in close collaboration with the data analysis software team. It is important that these provisions are seamlessly implemented, and that the logic is thoroughly researched.

Comment 4.7 and Recommendation 4.8 from the October 2003 EFAC report continue to reflect the sentiments of EFAC regarding these important issues. We look forward to learning about a comprehensive management plan for data analysis software development at the fall 2004 EFAC meeting.

5 Letters of Intent for New Instrumentation

5.1 Letter of Intent for USANS

In response to comments on the original letter of intent in their October 2003 report, EFAC received a revised letter of intent from an IDT assembled to propose a time-of-flight Ultra-Small-Angle Neutron Scattering (USANS) instrument. M. Agmalian, a pioneer in the development of the USANS technique for neutrons, presented a conceptual design for building the instrument on a shared beam line, and showed data from existing instruments in order to make a scientific case for the instrument.

Small angle scattering of X-rays and neutrons is routinely used to characterize structures on the nanometer to micrometer length scales. Extension to longer length scales is prohibited by low resolution and signal to noise in conventional instruments. In the 1960s Bonse and Hart introduced a novel monochromator design that overcame these problems with X-rays, and in the late 1990s Agmalian and co-workers successfully adopted the Bonse-Hart technique for neutrons at HFIR. The technique has since been implemented on the BT5 perfect crystal SANS at NIST to create the current world's best USANS instrument.

The new conceptual design for a TOF-USANS permits placing the instrument on a shared beam line by inserting a pre-monochromator of bent Si(2,2,0) in the main beam, which, according to calculations by the IDT, allows ~95% of the neutrons to pass through to the downstream instrument. Although the LOI suggests that the instrument could be accommodated at various SNS moderators, coupled H_2 or 25 mm poisoned H_2O are preferred. It is interesting to note that only the Si(220) reflection benefits from coupled H_2 while the six higher resolution reflections do best with 25 mm poisoned H_2O. The latter moderator also happens to be in less demand by other SNS instruments. The effects of the pre-monochromator on the transmitted neutron spectrum as well as the space requirements of the USANS instrument along the beam line would have to be considered carefully when pairing TOF-USANS with another instrument. To accommodate the TOF-USANS instrument in the limited space close to the source one might consider adopting a vertical scattering plane and placing the instrument above the chosen beam-line.

Data from existing instruments clearly demonstrate the utility of USANS for elucidating the morphology of large scale, polydisperse structures ($Q \sim 10^{-5}$–10^{-3} $Å^{-1}$), especially when combined with conventional SANS ($Q > 10^{-3}$ $Å^{-1}$). A TOF USANS instrument can collect data using several different reflection orders of the channel cut monochromator-analyzers. Because the Darwin width and hence the resolution width decrease dramatically with increasing order, the gap between conventional SANS and light scattering can be bridged in a single TOF-USANS experiment.

The performance gains over a reactor based USANS instrument are difficult to quantify due to the different modes of operation. At a given angular setting of a TOF USANS instrument, not all monochromator orders will in general produce useful data due to the vastly differing angular resolutions and count rates. For example at a scattering angle of 0.5 arcsec only reflections of order n=4, 5, 6, and 7 will be able to reject the direct beam. Moreover, the counting time required at any given angular setting will generally be dictated by the highest order reflection of interest. For example the efficiency of the n=7 data stream is down by almost three orders of magnitude compared to the n=4 data stream considering both the lower flux on sample and the smaller acceptance angle of the analyzer. While several reflections are likely to be useful at any given setting, the total flux on sample probably does not accurately reflect the useful data rate for a TOF-USANS instrument as compared to a CW-USANS machine.

If one considers simply the Si(440) reflection then the TOF USANS data rate will be 67% of the NIST USANS data rate at comparable resolution. However, there is a bonus of simultaneous access to 6 other reflections with a range of different resolutions and wave lengths. The coarser resolution Si(220) reflection for example will have 30 times the NIST USANS data rate with three times coarser resolution and it will thus provide an effective bridge to the conventional SANS regime. While more detailed and specific analysis will be required to provide an accurate comparison of these different types of instruments, it appears that easy access to a range of different resolutions and an order of magnitude smaller $Q_{min}=2\times10^{-6}$ Å^{-1} will be the main advantages of TOF USANS.

As opposed to other instruments that EFAC has previously evaluated, USANS is a relatively young technique that has yet to prove its scientific importance. The NIST USANS machine for example remains undersubscribed and there have only been 4-5 peer reviewed USANS papers per year over the last five years. To gauge the scientific potential of USANS, EFAC solicited referee reports from prominent members of the SANS community. The information provided to the referees was the LOI and the article by Schaefer and Agamalian. Five referee reports were received and anonymous verbatim copies of these reports are attached. All the reports were very positive indicating a considerable excitement in the SANS community about the future scientific potential for USANS and in particular USANS at the SNS.

5.1 Recommendation: The USANS LOI for a shared beam-line instrument should be accepted and the IDT should be encouraged to develop a full proposal. Such a proposal should include performance simulations for typical experiments and it should fully specify conditions for a down-stream partner instrument.
5.2 Recommendation: SNS should search for appropriate beam line partner instruments for a TOF-USANS machine among LOI approved instrumentation projects.

Collin Broholm

From: [redacted]
Sent: Friday, May 21, 2004 6:17 PM
To: broholm@jhu.edu
Subject: Advice regarding a proposed USANS instrument for the SNS

TO: Professor Collin Broholm
Chair, SNS Experimental Facilities Advisory Committee

Dear Professor Broholm,

I am responding to your request on behalf of the Experimental Facilities Advisory Committee (EFAC) of the Spallation Neutron Source for help to evaluate the letter of intent for a proposed new USANS instrument at the SNS. I believe that the construction of such an instrument could significantly maximize the long-term scientific impact of the SNS for the reasons set out below in response to your specific questions:

(i) Potential scientific impact:
Will USANS provide unique and important information on length scales from 0.01 to 100 micro-meters that warrants allocation of part of an SNS beam line plus the resources to build and operate the instrument?

In most cases, USANS will be used to extend the Q-range of companion SANS measurements to a lower Q regime, hence to larger microstructure sizes. The "unique and important" case is essentially the same as that for SANS in general: a statistically-representative quantitative measurement of the microstructure is readily obtained over many length scales. This is different from microscopy and other imaging techniques that give complementary qualitative (and local) information. While some of the more advanced imaging techniques, e.g., x-ray microtomography (XMT), provide data in electronic form that in principal can be analyzed to obtain some of the same information as SANS, in practice this involves the manipulation of extremely large datasets, and involves image interpretation that is frequently controversial. The final result obtained is based on significantly smaller sampling volumes than are possible with SANS, and is arrived at only after significant image-data manipulation. By contrast, SANS provides quantitative and statistically-representative microstructure information naturally, i.e., without the manipulation of large datasets. When USANS is combined with SANS, microstructure can be quantified (on an absolute scale) in a contiguous scale range from nanometers to many micrometers. No other method exists to do this. SAXS and USAXS methods get from nanometers to a little over a micrometer but USANS goes more than a decade lower in Q and gets into the tens of micrometer regime. Furthermore, a SAXS sample must generally be at least 10 times thinner than the corresponding SANS sample. While light scattering can compete with the USANS Q-range and size-range, it can only do this for samples that are transparent. Recently, I have used the NIST USANS for contrast variation studies aimed at distinguishing between calcium hydroxide (CH) and calcium silicate hydrate (C-S-H) gel structures within hydrating cement systems. The coarse CH contribution could only be resolved with USANS as it is too large for USAXS. I will report on this work as part of the paper that I will present at the upcoming ACNS meeting. The complex heterogeneous nature of cement leads me to believe that this problem was only solvable using USANS with contrast variation. No other technique would have provided the statistically-representative solution sought. In general, USANS provides the means to quantify the coexistence of nanoscale and mezoscale features: a major requirement for many emerging aspects of nanotechnology.

The case for USANS at SNS must be put in the context of SANS in general at SNS and HFIR. I recognize that fewer than 15 SNS instruments have been approved to date for construction. In these circumstances, I understand the reluctance to dedicate an entire beam port to an USANS instrument. However, I feel that the current plan to use part of a beam for USANS should be supported, provided a suitable instrument can be identified for the remainder of the beam port. This instrument, and its partner (which needs to be identified without delay) need to be seriously pursued at this time, or options will close as beam-ports are filled up.

(ii) Would there be a vibrant and scientifically productive group of users for such an instrument?

The USANS community is only just forming, following the revolutionary step advance in performance of new USANS instruments around the world, arising from the innovative work of the main PI of this proposal. However, decisions must be made now if the right instrumentation is to be in place by 2008. USANS would greatly enrich the SANS program at ORNL and make the SNS much more attractive to the SANS community, which otherwise remains largely centered at reactor facilities. The SNS time-structure may needs to be fully exploited in the detailed design (in addition to using multiple-order Bragg peaks) in order to give this USANS instrument the cutting edge it needs. However, present trends suggest that the omission of USANS from the ORNL neutron portfolio could be a serious mistake.

(iii) Technical viability of the instrumentation concept and the performance comparison to existing USANS instruments at steady state sources:

Others are better qualified than me to assess how the USANS could fully exploit the SNS pulsed source. I note that the use of many (but discrete and defined) neutron wavelengths would enable multiple scattering issues to be detected and mitigated (through use of appropriate algorithms). Clearly, the effective counting statistics can also be greatly enhanced by using the multiple peaks. The "first-principles" nature of the proposed instrument, when coupled with different target moderator characteristics, might enable new SNS developments to be explored, as well as offering scope for a range of specialized USANS applications such as stress analysis within thin films. In this connection, I note that this proposal has brought together one of the world's leading innovators in USANS development (M. Agamalian) and the active participation of one of the world's foremost innovators in pulsed neutron source target / moderator design (J. Carpenter). This fact, alone, is an extremely powerful endorsement for the need to proceed with this instrument's construction at the present time; such a combination of talent and interest will not be available if USANS development at SNS is significantly delayed.

I hope these comments are useful and will assist the EFAC in developing a final recommendation to SNS.

Regards,
[redacted]

[redacted]

[redacted]

Collin,
Since I am a member of the IDT, and the USANS community at large, my views are bound to have some bias. I'll attempt to respond fairly. I like to respond first to the technological advantages of the TOF-USANS over reactor based USANS, and than to the scientific basis.

Technological basis:
The TOF USANS instrument will be able to measure with both high and ultra-high resolution from up to seven reflections as shown in fig. 6 from Letter of intent (LOI). When the analyzer is rotated to angle θ, the q measured by order N is

$$q_N = N\, q_1$$

Since the measurement range from order 7 is limited to 2e-6 < q < 2e-5 _$^{-1}$, the 1st,2nd, and 3rd orders will all be measuring the direct beam. Thus not all orders are likely to produce usable data at the same time.

The strength of scattering will also determine how many orders can be measured on a given sample. I expect for the majority of samples, the 6 and 7 orders won't be used. All data having q > 1e-4 _$^{-1}$ will be collected primarily using the first order. The higher orders will be used to collect data only at q < 1e-4 _$^{-1}$.

The definition of q_{min} used in LOI is

$$q_{min} = (2\pi/\lambda)2\delta D$$

Using the above definition, the NIST USANS has q_{min} = 19.7e-6 _$^{-1}$. This resolution lies between the 2 and 3 orders of TOF-USANS. Conceivably, a reactor based USANS could be built to higher resolution than NIST-USANS. For example, if placed on a graphite hot-source (T=2,000 K) to use λ = 0.7 _, and if high index Si(991) channel-cut crystals were obtained, a reactor instrument with potentially similar flux to orders 6th and 7th could be built, with q_{min} = 2.5e-6 _$^{-1}$. The main advantage of the TOF-USANS is **both** ultra high (orders 6 and 7) and high resolution (order 1) can be achieved on the same instrument.

For most SANS experiments, a range in q-resolution is needed. Lower resolution is used to measure weaker scattering at larger q. On a pinhole SANS, the collimation is changed by moving guides in/out and the detector to achieve flexibility in resolution. The new TOF-USANS will be better able to provide flexibility in resolution, and cover the intervening gap (1e-4 < q < 1e-3) than NIST USANS primarily with 1st order. the 2nd and 3rd orders will achieve current (NIST-USANS) resolution, and 4-7 orders will measure to even smaller q depending upon the sample to be studied.

It is important to clarify how much higher will the detector countrate (C_D) be for 1,2 and 3 orders on TOF-USANS versus NIST USANS. I thnik there is an error in LOI calculation of the "performance gain factor". For the case of infinite slit smearing,

where A is the sample area, ϕ_S is the beam flux at the sample, dΣ/dΩ(q) is the macroscopic scattering cross-section of sample, and δD is the Darwin half-width. For infinite slits, the vertical resolution cancels with smearing correction. [In part 3 of LOI, they used the Darwin width squared, which I believe is incorrect. The flux at sample already has incorporated the other dependence upon Darwin width.] The gain in countrate of TOF-USANS over NIST USANS can be calculated from product of beam flux times Darwin width $\phi_S\delta D$.

	ϕ_S	$2\delta D$	Gain
NIST-USANS	17,000 $cm^{-2}s^{-1}$	1.54 arcsec	------
TOF-USANS			
order=1	105,000	7.00	28.1
2	11,000	1.60	0.67
3	1,300	0.61	0.03

For q > 1e-4 _$^{-1}$, The TOF-USANS will have a detector countrate **29 higher** than NIST USANS.

Scientific basis:
Based upon current use of the NIST USANS, a significant fraction (~1/2) of experiments could utilize higher resolution. (plasma spray coatings, clays, portland cement, many gel systems...) Just as significantly, higher count-rate at q > 1e-4 _$^{-1}$ would be a significant improvement, in achieving overlap with capability from pinhole SANS. The lower wavelengths will also help minimize multiple scattering, which becomes more important as you go to smaller q.

Currently, the NIST USANS instrument is slightly under subscribed. I believe it will be several years yet before we will have to deal with over subscriptions of factors of 2-3 typical on the pinhole SANS instruments. There are several reasons for this. 1) Although slit smearing/desmearing is easily handled, users from the SANS community must be trained on this matter. The easier to use GUI type software being developed will help in this regard. 2) For a number of samples, the jump in resolution from pinhole SANS (q_{min} = 1e-3 _$^{-1}$) to USANS (q_{min} = 2e-5 _$^{-1}$) is too large, the samples don't scatter strong enough to be seen. This, combined with the lower sample throughput (2-3 samples a day for USANS versus 10 or more for SANS) has discouraged a number of users. The factor of 29 gain in count rate from 1^{st} order of TOF-USANS would help greatly in this regard.

I can also discuss any of this with you personally, [redacted]

Collin Broholm

From: [redacted]
Sent: Tuesday, May 25, 2004 6:22 PM
To: broholm@jhu.edu

Collin:

I have looked over the letter of intent regarding a TOF-USANS instrument for the SNS. In my opinion access to such a device will add significant value to the small-angle scattering community, and at a rather modest cost in neutron flux and capital expenditure. USANS bridges one of the most important structural length scale regimes, connecting SANS and light scattering. Many materials science and engineering problems, particularly those relating to soft materials, will be influenced by access to this equipment. I support a recommendation to develop a full proposal.

[redacted]

Collin Broholm

From: [redacted]
Sent: Tuesday, May 25, 2004 3:08 AM
To: broholm@jhu.edu
Subject: Re: request for your advice on a proposed USANS instrument for the SNS byMay 25, 2004.

Dear Dr. Broholm:

I would like to strongly support the virtues of a USANS instrument at the SNS. Most of soft materials and living organisms have hierarchical structures in the length scale of 0.1 nm ~ 1 mm. The structures in the length scale shorter than a few 100nm are relatively well-explored by small-angle neutron (SANS) and X-ray scattering (SAXS). The structures in the length scale larger than a few 100nm can be explored by light scattering, if systems are translucent. However there are many systems which cannot transmit light beam because of too much turbidity, and too much light absorbance. There are many systems whose higher-order or large-length-scale structures have been left unexplored.

Roles of these higher-order structures or large-length scale structures on properties and functionalities of soft-materials or on activities of living organisms have been left unsolved. Cooperativity among different level structures in hierarchical structures has also been left unexplored, despite of its scientific significance. I hope USANS instrument for the SNS will give a strong impact to unveil these problems described above.

I believe that the USANS instrument at the SNS give a strong impact to break through the black box described above, and that clarification of the black box is scientifically and technologically very important. Moreover USANS technique has its own advantages inherent in using neutron beam as an incident beam, such as (i) contrast-matching technique to see particular components or particular phases in multicomponent-multiphase systems, (ii) small radiation damage of materials or organisms compared with high flux X-ray beams, and (iii) large transmittance of neutron beams against materials.

Finally I would like to point out that I am not in a position to give technical comments for the instrumentation itself. However, I believe the USANS which can correctly detect scattering on length scales from 0.01 to 100 micro-meters will provide unique and important information both scientifically and technologically.

With best regards,
[redacted]

>Dear [redacted]
>
>The Experimental Facilities Advisory Committee (EFAC) of the
>Spallation Neutron Source would greatly appreciate your help in
>evaluating a letter of intent for a possible new instrument at the
>SNS.
>
>The attached confidential material describes an Ultra Small Angle
>Neutron Scattering instrument and the science that could be
>addressed by it. To help maximize the long term scientific impact of
>the SNS we would greatly appreciate your opinion of the virtues of a
>USANS instrument at the SNS. We are mostly interested in your

>estimation of the potential scientific impact. Will USANS provide
>unique and important information on length scales from 0.01 to 100
>micro-meters that warrants allocation of part of an SNS beam line
>plus the resources to build and operate the instrument? Would there
>be a vibrant and scientifically productive group of users for such
>an instrument? Comments regarding the technical viability of the
>instrumentation concept and the performance comparison to existing
>USANS instruments at steady state sources would also be of great
>interest. As you will see this is the second application by this
>group. Your response will be used by EFAC to develop a final
>recommendation to SNS.
>
>Your response can be informal and brief and would be most helpful if
>transmitted by email to <mailto:broholm@jhu.edu>broholm@jhu.edu no
>later than Tuesday May 25, 2004. If you don't have time or there is
>a conflict of interest, we would appreciate an early indication of
>that and your suggestions for alternate referees. EFAC may transmit
>excerpts from your response anonymously to the Principal
>Investigators. Please let me know if you would prefer us not to do
>that.
>
>Sincerely
>Collin Broholm
>Chair, SNS Experimental Facilities Advisory Committee
>
>
>==
>Professor Collin Broholm
>Department of Physics and Astronomy
>Johns Hopkins University
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<<NEW ADDRESS>>---

[redacted]

Collin Broholm

From: [redacted]

Sent: Tuesday, June 15, 2004 10:11 AM

To: broholm@jhu.edu

Subject: RE: request for your advice on a proposed USANS instrument for the SNS by May 25, 2004.

Dear Colin

First of all I must apologise for the particularly unhappy set of circumstances that have led to my very late response to your request for some feedback on the proposed USANS instrument for SNS. I hope my comments are still of some use.

I turned to the task of evaluating the proposed USANS instrument with some prejudice. As Chairman of the Instrument Subcommittee at the ILL I have received, over the years, several proposals for USANS instruments which have all fallen short of support largely because the proposers were unable to identify a sufficiently active and extensive user base and corresponding scientific demand to warrant the necessary financial and technical commitment. Moreover, as a neutron scatterer of some thirty years experience in SANS at both ISIS and ILL, and as a member of the team that built ISIS in the early 1980's, I have always been convinced that SANS is better performed at an optimized cold source at a reactor facility than at a pulsed source.

Nevertheless, I have found the arguments presented in the documentation (ie the revised letter of intent and the paper by Schaefer and Agamalian) both erudite and compelling. The development and extension of the Bonse-Hart USANS technique to multi-wavelength time-of-flight operation has been carefully considered and evaluated, and although I find the resulting estimated count rates somewhat surprising, I can find no reason to dispute the calculations. It appears to me that the gain over similar instrumentation at existing reactor facilities is a real one, and is certainly sufficient to warrant the proposed design being taken seriously. In this respect I believe the proposed instrumentation to be technically viable. The only comments I would like to make regarding the instrumentation are as follows:

(i) The USANS instrument has an essentially open geometry. Have appropriate Monte Carlo simulations been carried out to evaluate the potentially large background, both secondary and direct, that might result from this open geometry?

(ii) The instrument as shown requires at least 3-4m of instrumentation orthogonal to the incident beam line at a distance of only 12m from the source. Is this feasible given the geometric constraints of the SNS? Might this pose shielding problems (as noted above)? Could the USANS beam line be extracted vertically from the direct beam?

(iii) Given that the all the Si monochromators are operating close to the backscattering geometry might it be worth considering cooling the monochromators (a) to reduce the reflectivity loss due to Debye-Waller effects and (b) to reduce any thermal diffuse scattering which could affect the intrinsic resolution function

The proposers have been thorough in their design considerations so I expect they may well have already considered some of these points.

Whilst I am entirely comfortable with the technical specifications of the USANS instrument (if some consideration is given to the points I have made above), I find my scientific prejudices a little harder to overcome. Whilst I agree with the authors that many SANS results are handicapped by the severe limitations placed by the lower Q-limits of existing instrumentation, I am also aware from my own experiences and those of others that it is not always entirely useful to approach smaller Q as there is a growing number and diversity of independent phenomena that contribute at the ultra-low Q range, and the separation of these phenomena is often intractable in all but idealized model systems. In addition it is often possible (at least in crystalline materials) to characterize the (eg size, shape, strain) parameters measured by USANS through inspection and/or Rietveld refinement of high resolution Bragg peaks (which can also independently provide such parameterization on multiphase, multicomponent samples, for which the USANS signals are superimposed).

However, USANS is a relatively new and unexplored technique – there may be much science to be accessed at these low Q values. Moreover with the flux gains proposed here the technique will undoubtedly cross an intensity threshold which may enable entirely new science to be carried out. In this respect SNS would undoubtedly be the centre of gravity for such studies.

In conclusion therefore, I would suggest that the proposed USANS instrument is both technically feasible and an exciting development and it could be built at SNS. Whether it should be built depends upon a careful evaluation of the existing and prospective user community and the science and technology they wish to bring to the instrument.

I hope these comments are useful, despite their late arrival for which I apologise deeply

Very best regards

[redacted]

[redacted]

[redacted]