The Neutron Advisory Board (NAB) met in Oak Ridge 27-28 March, 2014. Present were Gabriel Aeppli, Robert McGreevy, Yujiro Ikeda, Andrzej Joachimiak, Bernhard Keimer, Joël Mesot (Chair), Sunil Sinha, and Douglas Tobias. Not attending: Meigan Aronson, Sharon Glotzer, Andrew Harrison, John Hemminger, and Janos Kirz.

1) Charge

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

Charge

Neutron Advisory Board

2014

Based upon the central discussions of last year's meeting of the Neutron Advisory Board (NAB), the long-wavelength and short-pulse characteristics of the Second Target Station (STS) were established. This decision allows the Neutron Sciences Directorate (NScD) to select a set of world-class instruments that will best utilize these source characteristics. The NScD science strategy and recent workshops in quantum condensed matter and biology have identified key science problems that can be addressed by utilizing the STS, in conjunction with advanced neutron technologies, to deliver transformative capabilities for neutron science. NScD plans to expand its knowledge base in neutron source optimization, beam optics, spin-encoded scattering methods, computation, and other technologies in order to push the limits of the length and time scales accessible by the STS. For the upcoming meeting, we will propose a set of instrument concepts for the STS and seek advice from the NAB on making the critical decisions that will allow us to move forward with more detailed research and development of these concepts. In addition, the current status, recent science output, and instrumentation development plans at SNS and HFIR will be presented for discussion. We look forward to lively discussion on these topics at this year's NAB meeting.

Ron Crone

At the meeting a set of questions to be answered by NAB were raised by NScD (see appendix A):

1) Where should we strengthen priority areas?
2) Choose 5 instruments for STS and TDR
3) Are our HFIR/FTS priorities right?
4) Where should we target development?
5) How to engage community?

2) Meeting Agenda and Outcomes

An agenda for the meeting was developed by Ron Crone, Alan Tennant, and Robert McQueeney, in consultation with Joël Mesot and Meigan Aronson (see Appendix B).

NAB thanks Ron Crone, the active NScD director, as well as all involved staff in the preparation of the meeting.

The meeting started with a welcome from ORNL Deputy Director Ramesh Ramamoorthy, followed by a review of the year's progress by Ron Crone, Alan Tennant and Robert McQueeney and a presentation of Ken Herwig on STS technical development's issues.

The second part of the meeting dealt with three sessions related to future scientific plans for FTS, HIFAR and STS. Research trends, as well as related foreseen instrumental developments were presented for the fields of 1) Biology and Soft Matter, 2) Quantum Condensed Matter, and 3) Chemical and Engineering Materials.

Remarks on the 2014 charges to NAB: through the evolution of the meeting it became clear to NAB that the above-mentioned charges could not be fulfilled. On one side NAB was presented with an enormous amount of information, including for example proposals for more than 20 new instruments at FTS, HFIR and STS. On the other side, essential benchmarking studies with other neutron facilities and even more essential with competing techniques were very lacunar.

Based on this observation NAB decided to focus on mainly 2 issues:

1) Actual performance of FTS and HIFR and

2) Identification of megatrends for future research neutron activities, in particular in view of STS.

Accordingly, a set of overall recommendations was put together. More detailed recommendations on the sessions ‘Biology and Soft Matter’, ‘Quantum Condensed Matter’, and ‘Chemical and Engineering Materials’, as well as on ‘STS target/moderator concept and R&D needs’ can be found in sections 4-6, respectively 7.

NAB discussed as well intensively the succession of K. Beierschmitt and is of the opinion that a strong scientific leadership is urgently needed. NAB therefore recommends accelerating the search process.

3) Overall recommendations:

3.1 Recommendations for a smooth running of future NAB meetings

For future meetings, NAB requests the overall financial, staffing and performance figures to be presented by the head of NScD, as well as an organizational chart.

NAB requests as well a short written answer to the points raised in its previous meeting report. This should occur within 6 months after completion of the report by NAB.

In order to be able to set priorities, as often requested in the charges to NAB, benchmarking against leading competing facilities, both at the level of facilities and instruments will have to be provided.

3.2 Overall performance of FTS and HFIR

Upon NAB requests more detailed information on various indicators was made available by the NScD directorate.

3.2.1 Machine:

Beside issues related to last year target’s failures and for which solutions are currently been worked out, the performance of the accelerator is excellent. Nonetheless, especially in view of the advancing age of the SNS complex, a good balance between accelerator/source developments/maintenance, accelerator/source operation and instruments operation needs special attention from the NScD directorate.

3.2.2 Scientific impact:

NAB is impressed by the development of Neutron science at SNS and HIFR. Indeed, outstanding results have been presented in all major science topics. The increasing number of publications and more importantly the fact that more than 10% of those are in high impact journals is a healthy sign. NAB is expecting further improvements in output efficiency to be presented at future NAB meetings.

3.2.3 Organization

From various presentations it became clear that the staffing situation on the instruments has improved. In the past two years, internal reshuffling of resources allowed the staffing on instruments open to users to reach international standards. NAB congratulates NScD for this achievement and expects such standards to apply as well to instruments recently commissioned

NAB is looking forward to the first highlights resulting from these new capabilities. The next 2-3 years will be crucial to demonstrate the relevance of neutrons in the extremely competitive field of protein crystallography.

3.2.3 FTS and HFIR: medium term developments

NAB supports the plans for a full completion of the existing instruments in order to both 1) fully exploit the potential of these instruments and 2) create new science capabilities.

NAB feels that priority has to be given to the following instruments: MaNDi, PowGen, CNCS. Largest gains in performance can be achieved through a full detector coverage of these instruments. In view of the sensitive situation regarding availability and cost of 3He, NAB wishes regular update reports on detector developments.

3.2.4 User communities

NAB considers essential for the success of neutron science at ORNL, to continue the building of user communities, with a particular emphasis on the fields of chemistry and biology. This could be achieved for example through the establishment of a close relation with a prominent soft-matter/bio/chemistry scientist. Finally NAB recommends to strategically develop in-house research programs which act to attract US potential user communities from outside ORNL.

3.3 STS, FTS and HFIR: long term development

3.3.1 Megatrends

Following last year's NAB recommendations a number of scientific workshops aiming at defining the long-term strategy of the NScD directorate have taken place. NAB is looking forward to the reports resulting from these scientific workshops, some of which remaining to take place. While more detailed recommendations on the 3 main scientific topics can be found in the subsequent sections, the following overall recommendations can be made:

NAB has identified a few Megatrends that should serve as a basis for the development of scientific cases for NScD in general, and toward the realization of STS in particular:

1) Computing capabilities as enabling tool

2) Polarization capabilities , manipulation of spin degrees of freedom

3) Advanced concepts for optical and guide components

4) Progress in sample environment

In the past few years technical breakthroughs have been realized in each of these areas. NAB is of the opinion that a successful integration of several (ideally all) components into the concept of future neutron beamlines will be essential to address the complexity of the Grand Challenges facing our society. USA is currently in the unique situation to master most of these technologies, and as such ideally positioned to further strengthen its leadership.

3.3.2 High priority research fields

More specific to the neutron science division and ORNL, NAB identified the following promising new directions

•DNP for both biological studies and neutron polarization

•Chemical reaction dynamics

•High magnetic fields in collaboration with HMFL

•Time-dependent reflectometry

•High resolution powder diffraction

• Online modeling

In all these fields, ORNL has the potential to lead a US-wide effort.

3.3.3 Long term strategy: what remains to be prepared?

First ideas for the long term of neutron science at ORNL have been presented. Some were very mature, others at a very speculative stage. NAB recommends the following steps for each proposed instrument:

1) A scientific case must be completed and at least one 'smoking gun' experiment suggested.
2) Beyond rough estimates, complete computer simulations from the source to the detector must be realized.
3) Benchmarking against competing methods (X-rays, nmr, …) and neutron instruments at other sources should be performed.
4) Since a large number of new instruments is currently considered at all three neutron sources, it is essential for NScD to establish a clear procedure for the decision making process.

NAB is looking forward to the progress reports to be presented at future meetings.

4. Detailed report: Biology and Soft Matter

4.1 Overview of the division and its recent activities

The Biology and Soft Matter Division is organized into three groups: Biology and Biomedical Science; Energy and the Environment; and Structure and Dynamics of Soft Matter. The primary goals of the Division are to run an excellent user program and to become a unique center of neutron-based scientific excellence in biology/soft matter. The research priorities of the group include soft adaptive materials; membranes, thin films, and interfaces; fundamental interactions; bioenergy and biotechnology; biohybrid and bioinspired materials; and biomedicine. The research activities of the Division, especially in the area of biology, appear to be well balanced between NScD and the rest of ORNL, and it is evident that efforts to exploit obvious synergies between scattering measurements and computer simulations are underway.

Recommendation: The NAB had the impression that the majority of neutron scattering studies at ORNL in the areas of biology and soft matter are being carried out by ORNL scientists. Thus, the NAB believes that there is an urgent need to double down on efforts to attract a critical mass of new external users in these areas during the next couple of years. An important step in this direction is the Workshop on Structural Biology, Bio-materials, and Bioengineering that was held at UCSD in January, 2014.

Recommendation: The NAB recommends that the NScD attempt to recruit top-notch long-term visitors, e.g., a well-known structural biologist and/or polymer scientist, to serve as "ambassadors" to their respective communities, following the successful model of Collin Broholm in the Quantum Condensed Matter Division.

4.2 New opportunities for neutron science in biology and soft matter

The UCSD workshop defined the capabilities that will be required for neutron scattering measurements to make a significant impact on biological problems. These include: a broad suite of instruments capable of probing structure and dynamics covering a wide range of time and length scales (ps-ms, Å-mm), on crystalline, partially ordered (e.g., membranes), and solution samples. The ability to make the measurements on small samples is important in many applications. To make the most of the measurements, facilities for deuteration of biomolecules, both complete and partial ("segmental"), are necessary, and these, in turn, require advanced capabilities in plant and microbial biology. It is also clear that biology and soft matter are areas where multiscale computational modeling, carried out in concert with experiments, is indispensable.

Such capabilities will open the door for neutrons to provide key new insights into complex biological processes, such as cellular signaling, that involve the formation and dissociation of complexes between two or more biomolecules, some of which may undergo transitions between disordered and ordered states upon complex formation, as well as processes occurring in membranes, where lateral phase heterogeneity on the few-nm length scale plays important, yet poorly characterized roles.

Recommendation: The NAB called out computing capabilities as an enabling "megatrend" in science that should continue to be integrated into the current and future capabilities across the NScD. The NAB would like to hear about how computational modeling is being integrated into biology and soft matter research by NScD scientists and their collaborators at ORNL and elsewhere.

4.3 Current capabilities of instruments for biology and soft matter research

Biology and soft matter research at ORNL is currently served primarily by five instruments that are in the user program (Bio-SANS and GP-SANS for structural studies at HFIR, the TOPAZ single-crystal diffractometer at the SNS, and the CNCS and NSE spectrometers for dynamics measurements at the SNS). With the exception of NSE, all of these instruments are performing well and are meeting their design goals. The instruments appear to be staffed by appropriately trained scientific and support teams. The IMAGINE Laue diffractometer at HFIR was recently commissioned, and the MaNDi macromolecular diffractometer at SNS is presently being commissioned. These latter two instruments will give a much needed, major boost in capabilities in the US for macromolecular crystallography using neutrons.

Recommendation: In order to ignite the nascent interests of a potentially large user community of structural biologists, high profile studies that demonstrate the capabilities of the NScD macromolecular crystallography instruments, especially MaNDi, must be carried out and disseminated broadly within the next couple of years. It is also crucial that efforts to reduce data collection times on increasingly smaller crystals be continued.

4.4 New instrument concepts for biology and soft matter research

The presentations by scientists in the Biology and Soft Matter Division included concepts for new instruments at HFIR and the FTS and STS at the SNS that address many of the gaps in current capabilities at NScD facilities, including fiber and membrane diffraction, time-resolved measurements over multiple length scales simultaneously, spectrometers capable of accessing time scales up to 1 ms, and the ability to collect full macromolecular crystallography datasets in one day on small (~0.001 mm^3) crystals. A total of ten new instruments were mentioned.

Four were proposed for HFIR: MICROSE, a spin echo spectrometer for dynamics measurements on timescales up to 1 ms over a large Q-range; BARNS, a broad angular range neutron scattering instrument for time-resolved structural studies across a wide range of length scales in cellular substructures, tissues, and fibrils; ALIGN, a non-crystalline diffractometer for structural studies of partially aligned fibers and multilayer membrane systems; and cVENUS, a cold neutron imaging instrument.

Two new instruments were suggested for the FTS: VENUS, a multi-mode, wavelength-resolved imaging instrument, which is apparently already considered a high priority for the BES SING-III proposal; and SWANS, a unique high-resolution small-wide angle neutron scattering instrument with grazing incidence capabilities for characterizing structures from the submolecular to the nanoscopic scale.

Three new instrument concepts were targeted for the STS: T-LR, a kinetics reflectometer for fast measurements, including time-resolved studies, on surfaces and interfaces;

mmLR, a small sample reflectometer for spatially resolved surface studies of small area samples; and eWALD, an enhanced wide angle Laue diffractometer for structure determination of large proteins and complexes, including membrane proteins, with small crystal volumes

FlOODS, a SANS instrument optimized for localized structure/degree of disorder of segments, was suggested for deployment at either HFIR or the STS.

In addition, two new concepts for enhancing the capabilities of multiple instruments were presented: a SANS/reflectometry incoherent scattering filter, and DYPOL, a dynamic polarization device proposed for implementation on any crystallography beamline that makes use of the combination of polarized neutrons and polarized samples to maximize coherent scattering from hydrogen while minimizing incoherent scattering background, thus providing gains of up to 2-3 orders of magnitude.

Recommendation: The number of new concepts presented by the Biology and Soft Matter Division is obviously much greater that the number of new instruments that can be built in SING-III and the initial suite of instruments at the STS. The Division needs to engage their user communities to gauge interest, identify priorities, and build science cases for the new concepts that are deemed to best fill in the gaps in current capabilities.

Recommendation: The NAB was very excited by the DYPOL concept. In addition to holding great promise for being a true game changer by providing enormous gains to neutron crystallography instruments, it could open the door to a number of yet to be imagined new experiments that make use of the ability to manipulate spins. The NAB regards DYPOL as a high priority, and recommends that the required R&D be commenced as soon as possible, with LDRD support if possible.

4.3 Chemistry and Engineering

Good progress has been made in bringing new instruments into operation and building the community, science program and publications. Mail-in has proved very effective on Powgen, even leading to very rapid publications, and should be considered for other instruments (in all divisions). The demand from users shows that sample environment is as important as instruments – if you don't have the right capability you can't do the science whatever the instrument performance. So this should be a key feature of, and be properly costed into, the STS case.

It is not recommend that instruments, or parts of instruments, are moved from FTS to STS (again this applies to all divisions). The cost saving is generally small compared to the total cost of an instrument, and there is a much higher effective cost in the closure of the FTS instrument and loss of its science program before the STS instrument is fully operational.

4.3.1 Diffraction

The Anger camera detectors on TOPAZ and Mandi have only been in real use for a short while. It might be sensible to wait (at least a year?) until any possible residual design issues come to light before investing in more detectors for SNAP and TOPAZ.

There is a demand for sample environment at high pressure and low temperature. Since this is potentially cross-division a 'leader' should be identified.

The proposed RAPID diffractometer has to be a lower priority than the proposed POWGEN rebuild. However, given the now very productive Powgen program, the relevant effort should be prioritized so that Powgen is out of use for the minimum amount of time. In addition, it was not entirely clear how RAPID would overlap with the capabilities/uses of NOMAD.

As noted previously, HRPD is one of the most obvious priorities for STS.

4.3.2 Engineering

A test of texture measurement on NOMAD would be recommended to inform any future discussion of a new instrument in this area.

VENUS is, and has been for some while, an obvious priority for FTS. Previously it was considered that this would be funded through non-BES routes, whereas now it is mentioned as part of a SING-III. Have the other possibilities fallen through?

The VULCAN upgrade proposed would simply move the use of the instrument from one group of users to another, when even the existing potential demand is not satisfied. It should be considered whether an additional instrument is a better strategy. Now that NRSF is back in the user program its complementarity to VULCAN should be better advertised. And with regard to the use of NRSF, it may be advisable to (gently) enter into discussion with Chalk River as to where their successful industrial residual stress progam might move when their reactor ceases operation (as now seems highly likely after 2016).

This group has made no proposals for instruments at STS. Given the potential areas for future expansion of the neutron scattering user base, one might expect at least two of the STS instruments to be in the engineering area.

4.3.2 *Spectroscopy*

Early experiments on VISION are showing great promise. There is an urgent need now to build the user community that can exploit this. The lack of key sample environment when the instrument came into operation is a lesson for the future (as previously mentioned with regard to STS in general). The expected high use of DFT in conjunction with VISION experiments would provide an obvious focus (and very quick win) within the Centre for Advanced Materials Modelling. Is it possible to fit this into that project even though it is already underway?

The combination of both low-risk and highly innovative ideas for future instruments within this group was highly appealing. The more innovative proposals now need detailed simulations and possibly some engineering feasibility check.

4.4 Quantum Condensed Matter

4.4.1 Megatrends

Neutrons are different from photons produced by accelerators in that their increased potency is due not to orders of magnitude increases in flux, but rather by orders of magnitude improvement in their exploitation using advances from other fields. The decade of 2010 is no different than previous decades in such advances, yielding the following three major new capabilities which justify building STS:

- 1. Computational modelling revolution, uniquely matched to neutrons because of simplicity and weak-coupling nature of their interaction with condensed matter.
- 2. Control of spin polarisation - whether dynamically or with static fields - of electrons, neutrons, and nuclei, including particularly H and He3.
- 3. Optics revolution, including particularly metamaterial concepts as well as ever increasing fabrication skills, which have yet to be exported to neutron science.

Impacts of 1-3 will be in all areas from biological crystallography to quantum matter, and 1-3 should form the core of the science and technology case for STS, as well as the basis for program and instrument design.

4.4.2 Trends for Neutron Science @ ORNL

The NAB meeting was not structured so that we could provide significantly more detailed recommendations, although it is possible to make some other observations on QCM at ORNL at present and in the future:

- 4. There is a healthy, world-class programme in this field, as evidenced by numerous high profile publications as well as the hire of Alan Tennant as Chief Scientist and Collin Broholm as Scientific Consultant.
- 5. Extreme sample environments, involving high pressures, low temperatures and **high-magnetic fields** continue to define a frontier for this field, and are of highest priority for upgrades at FTS and HIFR as well as new facilities at STS. The NAB

was particularly intrigued by proposals for high-field magnets based on high-temperature superconductors, which should be further explored with the NHMFL in Tallahassee.

- 6. Instruments which further exploit the extraordinary ability of neutron detection to be multiplexed, as suggested by the ORNL scientists at the NAB meeting, are likely to lead to orders of magnitude gains in data collection efficiency in QCM as in all other areas of neutron science, and need to be built for neutrons to maintain their core position in QCM.

4.5 Comments and recommendations on the STS target/moderator concept and R&D needs

- Congratulations for convergent major parameters of STS target in terms of proton pulse mode, repletion rate, power (Short, 10 Hz and 500 kW) for long wavelength neutrons, which are of critical importance to start technical design study, meeting to request from the demonstrative neutron instrument for new science.
- There are several key technological issues to be solved before getting into the detailed design, time for R&D should not be underestimated and needs margin to have reasonable key technical bases for the challenging STS. The R&D has to be started as soon as possible.
- Concerning technical issues on STS target system for R&D, there are many common interests in the ESS project and also a proposal for the second target station at J-PARC. Given the importance addressed for the challenging concept, it is advisable to have a new collaboration dedicated to the concept of long wavelength and short pulse with high peak intensity.
- Key technical issues are solid target with extremely high energy density injection, search of the best coupling between the target core and moderator, concept of compact high brightness moderator concept validation, in particular identifying the function of pre-moderator/ including moderator material choice, etc.
- We fully agree with SNS on importance of experimental validation of the new concept on the target and moderator along with the neutron focusing guide optics.
- It is recommended SNS team establish R&D procedure as soon as possible

identifying specific technical issues, time-lines and places for experimental measurements.

- For moderator concept validation, small accelerator base neutron sources are highly recommended to use, LENS, Hokkaido Univ.
- Polarization, Chopper, High Magnetic field, High pressure, etc., all should be extreme from the currently achievable. Something different from conventional techniques has to be their baseline. (For example, a gain factor of 10,00 looks very attractive.)
- In order to examine feasibilities of those challenging techniques, existing test neutron beam lines are to be utilized. (For example, BL10 at J-PARC source with 25 Hz is available to apply.)