Report of the Neutron Technical Advisory Committee - 5 & 6 March, 2009

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Overview

Neutron scattering is an indispensible technique for studying the structure and dynamics of materials. Due to the difficulty of producing the large number of neutrons necessary, neutron methods are pursued primarily in large centralized facilities. Typically these facilities, often in partnership with other organizations, develop a variety of instrumentation, each optimized for making a particular type of measurement. Scientists from academia, industry, and government then apply for time to pursue their research agenda. The successful proposals are typically granted anywhere from 1 to 10 days, depending on the instrument and the type of measurement, to perform their experiment.

The utility of neutron scattering and the effectiveness of this operational model are widely recognized around the world. Several countries, including Germany, Australia, Great Britain, China, the United States, and Japan are building, or have recently built new or significantly upgraded neutron facilities. The two most powerful of these new sources are the Spallation Neutron Source recently commissioned in Oak Ridge, Tennessee and the Materials and Life Sciences Facility (MLF) at the Japan Proton Accelerator and Research Complex (J-PARC) in Tokai, Japan. These facilities promise unprecedented instrument performance for neutron-based research. Europe is contemplating an even more powerful international neutron facility.

Due to the large national and even international investment in the construction and operation of these facilities, it is important that they be designed to optimize the quality and quantity of scientific and technical results that these sources produce. The staff of J-PARC and the MLF has done an admirable job in this regard. The target and moderator systems promise superior performance, the instrument designs are impressive, and the device development activities are similarly world-class. Neutrons were first produced and recorded in the MLF on the 30th of May 2008. In June 2008, one of the first instruments, the Super High Resolution Powder Diffractometer (SHRPD) recorded the world's highest resolution neutron diffraction pattern. Measurements of the neutron flux show that its performance is almost exactly as expected, both in terms of pulse-width and intensity. By the 23rd of December 2008 seven instruments were sufficiently complete to be ready for commissioning and the decision was made to begin operating them in "friendly-user" or "pre-operations" mode. True user operations are not far away. Thus, despite some technical issues discovered in commissioning, the MLF is now poised to become one of the world's premier neutron facilities.

To realize this potential, however, the MLF must make the transition from a design, development, and construction project to scientific organization dedicated to user service and research excellence while continually improving the neutron instrumentation. The rest of this report is divided into sections concerning the transition to operations, comments on the instruments and device development activities, and issues with the target and moderator systems. Recommendations in each area are italicized.

Operations

While the target and moderator systems and the neutron instruments promise internationally competitive performance, user service must be provided at the same high level if the MLF is to produce the quality and quantity of science indicative of a world-class facility. International best practice for facilities running 200 to 250 days per year is > 6 staff per instrument (which includes technical support, sample-environment, laboratories, electronics, data-acquisition, data–analysis, and other direct user support activities). Because the current staffing level is ≈3.5 staff/ instrument, we believe that the number of users that can be served and the science that can be produced is limited by staffing.

> *NTAC recommends that, as instruments come on-line, staffing be increased to the level of about six per instrument consistent with international best practice.* *Furthermore, the MLF should endeavour to secure a credible commitment (or at least a plan) to staff and operate additional instruments at the proper level, at the time funding is sought to construct each additional instrument.*

To be successful, a neutron facility must provide a wide-range of sample environment equipment and laboratories for users to prepare their samples. However, apart from a very interesting high pressure development program and some efforts on a pulsed 60 T magnet, this is an area which need much more attention.

> *NTAC recommends that the MLF develop a comprehensive, prioritized list of existing and planned sample environment equipment for J-PARC (including equipment at JRR-3M that can be used at J-PARC) by the next NTAC meeting. In addition, a plan should be developed for the management of sample-environment equipment, including planned staffing levels and support space.*

As the type of equipment one requires depends critically on the types of users one seeks to serve, this will require that the MLF at least estimate the balance of scientific usage on each instrument. Desired service levels and space requirements can be developed by benchmarking against other leading neutron facilities.

Some soft matter users may run 20 or more samples per hour on a SANS instrument, and at a lesser but still significant rate on the reflectometers. As these samples are usually prepared at the facility, well-equipped user support laboratories very near the neutron instruments are essential for users in the areas of soft matter and biology. This space should be separate and in addition to the existing facilities for powders and other hard matter. Unfortunately, the current laboratory space in the MLF is wholly inadequate and the Ibaraki Quantum Beam Research Center is too far from the experimental halls to serve this function.

> *NTAC recommends that the MLF develop a prioritized plan for support laboratories at the MLF and/or accessible to users of the MLF by the next NTAC meeting. In addition, a plan should be developed for the equipping and staffing of these support laboratories.*

Many neutron facilities (SNS, ILL, ANSTO) have developed deuteration laboratories nearby that assist neutron users in preparing appropriately deuterated samples. This capability should also be considered for the MLF, but could be developed in collaboration with nearby universities or research institutes. In addition, the plan needs to include a well-organized system to check samples after irradiation and standard procedures to cope with activated samples. Presumably these activities will occur in the Class-I radiation laboratory.

Attracting industrial scientists is an admirable goal of the MLF. However, these users impose an additional set of requirements. For example, they require rapid access as industrial problems need to be addressed with a very short time line. They need secure office space and computer systems for proprietary research. And as industrial researchers are rarely neutron experts, they need a high-level of support from the staff. One important approach for educating this community is to produce attractive, interesting, and important results as soon as possible to show the power of J-PARC for solving industrial problems.

J-PARC also aspires to internationalize the use of J-PARC. They require that proposals for beam time be written in English and have put no limit on foreign users. However, simply making beam time open to all will not be enough. There should be targets for overseas usage, and an effort to create formal links when appropriate.

NTAC recommends that the MLF develop strategies for increasing the use of the neutron facilities by industrial and international scientists. This should include the types of facilities that will be required to attract these scientists as well as formal and informal outreach methods.

J-PARC will be a focus for some of the world's best scientists. Informal meetings and discussions are an important contributor to the scientific atmosphere in any research organization. These meetings often lead to new collaborations and result in significant advances in our understanding of materials and the development of new technologies for neutron science. These interactions are so important and exciting that certain areas at existing facilities are legendary as a highlight of the user's scientific experience. The committee did not see any location where these important interactions would naturally occur at the MLF. It seems to us that the Ibaraki Quantum Beam Research Center is too far from the MLF for informal scientific discussions to occur naturally. Moreover the Ibaraki Quantum Beam Research Center is on the other side of a very busy road which is difficult to cross safely. On a related note, J-PARC is located in the country-side. Thus the development of appropriate accommodations and restaurants are very important to attract users to the MLF.

Finally, one needs to measure success. The primary metric for any scientific organization is of course the quality and the quantity of the scientific and technical results. However to be successful, user facilities must also provide high quality "customer service" to an increasing number of users.

NTAC encourages the MLF (perhaps, in conjunction with the Japanese Society of Neutron Science) to develop a user-feedback system on the user experience at the MLF, so that improvements can be made in a timely and responsive way.

Instruments

The instrumentation development program at J-PARC/MLF is proceeding very well. Currently 15 instruments have either been funded or partially funded leaving only 8 positions for additional instruments. All 15 instruments should be operational by 2012. The instrument priorities have been set via a well-defined process which included input from the Japanese Society of Neutron Science. The following chart indicates the funded instruments and their status.

Name	Beamline Moderator	Description	Funding source	Status
4SEASONS	BL01 Coupled	High intensity chopper spectrometer	JAEA, KEK and Tohoku University	Operation/ Commissioning
iBIX	BL03 Coupled	Single Crystal protein diffractometer	Ibaraki Prefecture	Operation/ Commissioning
NNRI	BL04 Coupled	Neutron cross-section measurement	Hokkaido University, JAEA, Tokyo institute of Technology	Operation/ Commissioning
SHRPD	BL08 Poisoned (thin)	High resolution powder diffractometer	KEK	Operation/ Commissioning
NOBORU	BL10 Decoupled	Source characteristic and general test beam line	JAEA	Operation/ Commissioning
TAKUMI	BL19 Poisoned (thick)	Engineering diffractometer	JAEA	Operation/ Commissioning

iMATERIA	BL20 Poisoned (thick)	High Intensity Powder diffractometer	Ibaraki Prefecture	Operation/ Commissioning
NOP	BL05 Coupled	Fundamental physics	KEK	Construction/ Commissioning
H-Ref	BL16 Coupled	Horizontal geometry reflectometer	KEK	Construction/ Commissioning
HRC/VINS	BL12 Decoupled	High resolution chopper spectrometer	KEK, ISSP	Construction/ Commissioning
NOVA	BL21 Decoupled	S(Q) diffractometer	NEDO, KEK	Construction/ Commissioning
AMATERAS	BL14 Coupled	Cold neutron disc chopper	JAEA	Construction
HI-SANS	BL15 Coupled	High intensity wide-Q SANS	JAEA	funded
DNA	BL02 Coupled	Backscattering spectrometer	JAEA	funded
	BL11 Decoupled	High Pressure diffraction	JAEA, Tokyo University	funded

The balance among diffractometers and inelastic scattering instruments seems reasonable. One potential problem is that only 20% of the general purpose powder diffractometer (iMATERIA) is planned to be available for general user proposals. Another issue is that only two instruments for studying large scale structure (SANS & reflectometers) are currently being built. The only reflectometer was partially funded and has essentially been transferred from KEK rather than designed to take full advantage of the new source.

NTAC recommends seeking funding for the construction of a reflectometer that is optimized for the MLF with capabilities that complement those of the reflectometer transferred from KEK.

It is noteworthy that this instrument is next on the prioritized list developed in conjunction with the Japanese Society of Neutron Science.

On a positive note, the HI-SANS was recently fully funded with construction to begin shortly. We note that the capabilities of the HI-SANS instrument at J-PARC nicely complements those of the SANS machines at JRR-3M. Now the challenge is for the staff of MLF and JRR-3M to work together to educate the community to make the most effective use of these complementary capabilities.

By December 2008 seven of the above instruments were sufficiently complete to be ready for commissioning and the decision was made to release some fraction of their beam time to user operation. Over 100 proposals were received for this initial user run and 100 more have been received for the next period starting in May 2009. However many of these 7 instruments still require substantial effort to make them truly ready for user operations. Moreover as expected for such a large and complex facility, commissioning has thrown up new technical challenges: the accelerator power is lower and more unstable than hoped because of the problems with the RFQ and there are problems with the operation of the hydrogen circulators that need to be solved before the moderators can be run routinely.

> *NTAC recommends that at this early stage the MLF focus on commissioning instruments rather than hosting users.*

This will allow problems to be discovered and solved by the staff before users discover them. Early experiments should be chosen for not only the quality of the science, but also for ability of the instrument to produce quality data from the particular sample. All of this requires slowing the release of beam time to the user program in the near term. We also suggest focussing on a few high-priority instruments.

Many instruments are functioning at a fraction of their ultimate capabilities, not just because of accelerator problems, but rather due to the lack of funding for a full complement of detectors. In some cases, the detector coverage is a small fraction of the ultimate detector coverage. We realize that there is currently a shortage of ^{3}He on the world market, but feel that adding more detectors is a simple, cost effective way to boost instrumental performance.

> *NTAC recommends that the MLF develop a prioritized plan to acquire and install the full detector complement on all of the new neutron scattering instruments.*

Finally, we were quite happy that the MLF, as part of its long-term strategy, plans to replace or upgrade each instrument every 10 to 15 years. Such a renewal program is essential if the MLF is to gain and maintain international stature.

Devices

The device development activities at J-PARC, pursued in collaboration with laboratories/universities across Japan, are truly world class. During the transition from a construction site to a user facility the pace and diversity of this development will probably decrease, as focus is shifted towards finalizing the current instrument suite, commissioning these instruments, and delivering first scientific results.

> *NTAC recommends developing a long-term strategy for instrumentation and utilization and using this to identify the devices necessary to realize their vision. Then they should pursue, in collaboration with partners, developing the devices that cannot be procured elsewhere.*

Choppers

From the presentations and the tour of the facility it is clear that J-PARC is in contact with the leading suppliers worldwide for all the main chopper types. They are also involved in state of the art development of super mirror based - slit packages for Fermi choppers and - fast spin-flip choppers for signal-to-noise enhancement. The standardization of the touch panel control of these devices is also very commendable. For the operational phase J-PARC will need a small adequately staffed group responsible for operation, maintenance, repair and some new development of the these facilities. This activity is very much on track.

Optical devices

J-PARC collaborators, KURRI, RIKEN, Hokkaido and Tohoku, are all highly recognised for the development of neutron optical devices.

The MLF is equipped with state-of-the-art neutron guides – both in terms of coating and geometry. The numerically controlled polishing technique and high-*m* sputtering capability allow for the fabrication of short, supermirror focusing devices. These are well adapted to small samples or special sample environments and are impressive and very promising. These devices promise substantial gains in intensity on the sample and may also reduce background from the sample area. The very high quality of the polarising mirrors from the KURRI group allows for their use as a spin-flip chopper and in a MIEZE-type spin-echo setup.

Another interesting development is the development of "white-beam" focusing using magnetic lenses, which definitely will be interesting for SANS.

The development of polarized ^{3}He filters for white beam polarization using the SEOP method has shown good progress. ^{3}He polarisation of 60% in simple cells with lifetimes approaching 400 hours has been achieved. This development is very important for the long term polarization program at the MLF. However, substantial efforts are still required to develop cells which cover a wide angular range.

Detectors

Excellent progress has been made in detector development through collaboration with ISIS, ILL, KEK, Osaka, Tokyo and Kyoto. The development spans the range from long, linear PSD ^{3}He tubes (collaboration TOSHIBA), an improved version of the Engine-X (ISIS) scintillation detector for TAKUMI, the neutron imaging detector for iBIX and new fast scintillation monitors, which will all be extensively used in the current instrument suites, to a number of concepts for future use.

DAQ and software

With event recording, 100Mbit/sec TCP/IP data transfer rate J-PARC has developed a high speed, efficient, low power consumption data acquisition system, that will cope with the amount of data produced at the MLF. The chosen data format (NEXUS) also allows users access to the data using their own software. User friendly software is on the way and available for some applications on some of the experiments. However it is clear that it will take considerable time and effort until all instruments are adequately supported. This will need attention and adequate resources.

Target

The service life of the target shell is limited by radiation damage and/or cavitation erosion. Radiation damage is directly proportional to the number of kWh put on the target. However cavitation erosion is expected to increase with some power (up to 4th) of the beam power (power density). Also, it appears that there is a threshold below which cavitation erosion does not occur. This threshold is estimated to be about 400 kW of beam power at JSNS. As a consequence radiation damage will be the dominant damage mechanism during the initial power ramp up phase and will affect all three shells more or less equally. Also radiation damage leads to hardening of the material at a relatively early stage, which may actually increase the resistance against cavitation erosion. The current situation with the accelerator and the fact that the accelerator is likely to operate at relatively low power for a while provides the opportunity to learn about radiation damage in the MLF target. Of course, the longer a target is operated, the more one is able to learn.

In light of this and the fact that the SNS target has already reached 5 dpa with no indication of a problem, the NTAC believes that the limit of 5 dpa currently set for the target is too low. Note that the SNS target will reach 8-9 dpa by the end of the current running period and SINQ targets are regularly used up to even higher dpa levels - recently up to 25 in the steel cladding of the target rods (though not pulsed).

Radiation damage also leads to loss of ductility (less rapidly than hardening) which makes the material less resistant to impact. Impact is a consequence of the thermal expansion of the Hg and hence more serious on the target container, where it may enhance fatigue, than on the enclosure hull. Another impact-like load comes from the cyclic internal heat deposition in the container material and is about equal for all three walls (mainly compressive stress). Thus, even with only limited effects from cavitation erosion, failure of the Hg container will occur before the failure of the water-cooled shroud. The target is designed to cope with this. Moreover a post irradiation examination (PIE) on a target which has reached the end of its service life will yield more significant results than PIE on a target removed early.

Since PIE is going to take some time and the information will be the more useful the earlier it becomes available, the first target should definitively be examined (contrary to current planning). It should also be remembered that, once the pressure wave effect mitigation is successful, the criterion for exchanging targets will be radiation damage. Therefore it is important to obtain realistic information on this issue from examination of the water shroud of Target 1, even if it does not fail from cavitation erosion until 2012.

> *For these reasons and also in the interest of waste and cost minimization, NTAC recommends using the first target to the natural end of its service life, or at least to a radiation damage level well beyond 10 dpa and carry out a PIE as quickly as possible.*

This most likely means that it will have to be exchanged during a scheduled user run. So the users should be warned of this possibility at each run cycle.

Beam profile

The devices for measuring the beam profile work well and show that the beam profile has a symmetrical shape. However, damage on the target can be reduced by providing a less peaked intensity distribution to the target. This will extend the lifetime of the target again reducing costs and waste.

> *NTAC recommends that every effort should be made to provide a less peaked intensity distribution at the target than the present Gaussian one.*

A method should be developed which allows regular checks of the functionality of the leak detection system of the space between the hulls, e.g. a gas analysing system into which relevant species (Xe) can be introduced for validation purposes. A source of such gas may be available in the ballast tank of the mercury loop.

Laser Doppler Diagnostic System

The system currently being developed for measuring the vibrational behavior of the target shell under the impact of the proton beam is considered to be of value in two ways: (a) to judge whether or not the gas injection system is working properly and (b) to acquire information on the total damage potential of the beam applied. Once the gas mitigation system becomes operational and effective, this system will therefore still be an important diagnostic tool for securing the longevity of the target by monitoring the gas injection efficiency. Efforts to develop a reliable system are therefore endorsed by the NTAC.

Spare target

In the interest of minimizing waste and cost, the NTAC agrees with the plan not to use the spare target now being manufactured unless of course there is an unexpected failure of the first target.

Development of future targets

Thanks to the excellent efforts of the JAEA team there is now a relatively clear understanding of the mechanism of cavitation erosion in mercury and the measures required to mitigate it. The preferred solution is injection of gas bubbles with diameters less than 100 μm. Again, the group was successful in identifying a promising method to generate such bubbles (swirl bubbler). Testing its functionality under flowing mercury in the ORNL-Target Test Facility (TTF) is now a high priority. This development program relies on close collaboration with the SNS team.

> *NTAC believes that adequate funding for testing the swirl bubbler concept at ORNL is of paramount importance and will clearly pay off quickly.*

The design of the reduced size target as presented is still in a conceptual state and should be reviewed carefully before giving it out to a manufacturer for detailing. Apart from the question of how to arrange a bubbler system, there are other issues the Committee considers worth revisiting, such as leakage monitoring and capture, the attachment of the target nose to the spool piece (there are now tie-bolts on the spool piece, which may present a long-term risk). In this context it might be worthwhile to carefully analyze the concept developed for the ESS target (ESS- Technical Report Update, 2004). In addition, the nose piece itself may - apart from the general flow guide system - still need some improvements, *e.g.* to avoiding gas trapping (no flat horizontal surfaces) *etc.*

The present schedule for developing the reduced size target calls for fabrication to start in early JFY 2011 and installation in the first quarter of JFY 2012. Given the present difficulties with the accelerator system this might look overly ambitious but the Committee recommends not to relax this schedule in view of the fact that the spare target currently under manufacturing is not intended to be used.

Neutronic performance

The high-efficiency, coupled, super-critical para hydrogen, cold moderator with water pre-moderator is a signature feature of the J-PARC MLF. The diffraction data obtained on the Super High Resolution Powder Diffractometer transported from KEK indicates the superiority of the para-hydrogen. However, the comparison with the KENS methane moderator does not go far enough. Comparisons with the ISIS and SNS high-resolution diffractometers should also be pursued. The data is useful for evaluating the effectiveness of the para-hydrogen moderator and for giving a measure of the para to ortho ratio of the hydrogen moderators at existing facilities as well as for future moderator development.

Almost all of the integrated energy spectra observed at various beam lines are consistent with the simulations, showing that reliable calculations were performed and the construction of the TMRS was also performed precisely. However, there exist large difference at some beam lines, and the reason for this should be found as the process gives useful information on beam-line design and/or measurement procedures. The spectra obtained by C-TOF are not completely reliable, so the data obtained with the ^{3}He detector should be compared with simulations. Precise data obtained at low power are very important for understanding the neutronic performance at high power. Therefore, accumulation of spectral and pulse shape data is required at this stage.

The ortho-para ratio is a key parameter for the performance of the moderators, since all moderators were optimized assuming para-hydrogen, it may be necessary to redesign the moderators if the ortho-hydrogen ratio increases with the accelerator power.

> *NTAC recommends that the ortho-para ratio be experimentally determined, for example, by measuring the pulse shape of the decoupled moderator, by Raman scattering, and/or thermal conductivity.*

Spare moderators need to be fabricated. From a structural complexity point of view, the poisoned moderator is the most likely to cause problems. However only one instrument faces the narrow side of the moderator, and the performance of the decoupled moderator is quite similar to that of the wide side of the poisoned moderator. The coupled moderator is expected to be the most reliable. Even if problems occur with the coupled moderator, a decoupled moderator can stand in the coupled moderator for a while.

> *NTAC recommends that the first spare moderator should be a decoupled moderator with a decoupler material other than AIC. A new decoupler material is required as soon as possible.*

The MLF staff has been exploring replacing the light water in the moderator systems with D_2O. However, from the data shown it appears that the intensity gain from this change will only increase the intensity of the tail of the neutron pulse from the coupled moderator. Thus there is no apparent performance advantage in going to heavy water.

Cryogenic systems

Except for some trouble with the cryogenic pumps, the operation of the cryogenic systems is as anticipated. The shaft in the pump develops vibrations as the flange cools. These effects may be related and be caused by cooling of the shaft thereby increasing the gap in the air bearing. Thus both problems may be fixed by reducing the heat transfer to the shaft. However, the pump designed for He, now used at J-PARC may not be suitable to H. Alternatively, pumps with proven designs are available, and have been used for a long time at ISIS, LANSCE, and SNS.

> *NTAC recommends that consideration be given to switching to one of these proven designs in order to avoid further down times related to pump development.*

Hot cell entry

The MLF staff planned to reduce the radiation levels in the target facility by draining the mercury into a shielded container. However, radioactive isotopes were observed to stick in the pipes, resulting in much higher radiation levels than anticipated. Thus the MLF needs to develop a different way to enter the target area. The proposed iron shield is feasible for now but in the long term, it would be better to try to develop a filter system to remove the "sticky" elements. The NTAC recognizes, though, that such a filter may be difficult to install on the activated Hg loop.

Used component disposal

For cost-effective disposal, it is essential to reduce the volume of the radioactive waste. The scenario presented for cutting the used components is basically reasonable. However, the power up scenario has already been changed, and if the life of the target is further increased by adopting a larger dpa value than 5, the schedule should be adjusted. In the future, the effect of the pitting should also be taken into account in the schedule. Furthermore, solutions to the problems discovered in the early tests need to be developed. Additional experiments with the cutting device are key. The items of PIE should be discussed for future target improvement and diagnostics.

Concluding Remarks

The committee would like to extend their gratitude to the MLF team for their openness and clear, carefully prepared presentations and for their hospitality during our stay. It is clear that in terms of the source and instrumentation, the MLF will be an internationally competitive neutron scattering facility. We have every confidence that, with an appropriate level of support, they will be able to successfully realize their goal of becoming one of the world's premier neutron scattering facilities.