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Consultancy Meeting on Directionally Focused Moderators for Enhanced Neutron Beam Intensities to Support Materials Research and Applications

7-9 December 2010

IAEA, Vienna, Austria

Report of the IAEA Consultant Meeting

Vienna, Austria, February 2011

CONTENTS

1. BACKGROUND AND OBJECTIVES

1.1.Background

Moderated neutron beams are produced by a slowing-down and thermalization process, which suffers from very low efficiency. Indeed, only few neutrons which enter the moderator will appear in the useful neutron beam direction. The most inefficient step in this process occurs when neutrons are emitted from the face of the neutron moderator uniformly in all directions, and only the small fraction, that happen to be going along the neutron beamline, makes it to the sample position. One exception to this generalization is the “grooved” moderator concept, implemented at IPNS, ANL (USA), KENS, J-PARC (Japan), and TS2, ISIS (UK) in which neutrons leaving the bright “groove” surfaces in the wrong direction are scattered back into the moderator from the “fins” and get another chance to be usefully directed. However, even grooved moderators provide only a modest increase in the useful neutrons reaching the sample position. Clearly there is ample room for improvement.

At several facilities, research is underway to develop moderators which focus neutron beams in a preferred direction as opposed to emitting neutrons isotropically. For example, recently use of diamond nanoparticles for cold, very cold and ultra-cold neutrons revealed very promising results at ILL (France), where significant increase of the neutron brightness was observed for wavelengths above 7Å reaching a factor of 5 at 20 Å. Other similar studies are on-going at SNS (USA), J-PARC (Japan), ISIS (UK), and elsewhere. However, it appears that little communication is occurring among the involved teams.

Small scale accelerator facilities at Sapporo (Japan), Bariloche (Argentina) and LENS (USA) are collaboratively developing new moderator experiments and simulations to improve available cold neutron fluxes. The results are encouraging and need to be shared with larger spallation neutron sources and research reactors.

1.2.Objectives

The purpose of this consultancy meeting was to bring together teams from spallation neutron sources and research reactors working on theoretical, experimental, and engineering aspects of directionally focused neutron moderators. We discussed the state of the art, identified areas of needed research and development, and explored possibilities for collaboration. Specific objectives of this meeting included:

- Review various materials presently used or under development for advanced neutron moderators
- Discuss computer codes used to perform design and optimization studies of advanced moderators; their capabilities, availability, and necessary development
- Examine available data libraries and experimental data, identifying gaps in their coverage and proposing those actions necessary to fill in said gaps
- Propose dedicated validation experiments in support of modeling and engineering design efforts for advanced neutron moderators

While the overall objective of the meeting primarily addressed directionally focused moderators, both the hosts and attendees recognize that such considerations cannot be separated from general issues regarding advanced cold neutron sources. Accordingly, many of the presentations, discussions, and recommendations apply equally to these topical areas as well.

2. WORK DONE

The meeting was attended by 34 international experts from 18 Member States. This event overlapped (both attendants and agenda) with the third and final meeting of the IAEA Coordinated Research Project on Improved Production and Utilization of Short-Pulsed Cold Neutrons at Low-Medium Energy Spallation Neutron Sources. Ms Francoise Mulhauser, Scientific co-Secretary with Mr Danas Ridikas, both from the IAEA, welcomed the participants and outlined the goals of the Consultancy, and described the ongoing Research Coordination Meeting for the above-mentioned Coordinated Research Project. Each of the meeting participants introduced themselves, their institutions, and their connection to neutron source development efforts. The attendees nominated Mr Yoshiaki Kiyanagi as chairperson for the Consultancy Meeting, and Mr Erik Iverson as rapporteur.

The first day and the morning of the second day consisted of sessions on cold and directional neutron sources, shared between the Research Coordination Meeting and the Consultancy Meeting. The afternoon of the second day contained parallel discussions considering possible collaborations, distilling recommendations, and drafting summary reports for the meetings. On the third and final day of the meeting we merged the two groups for final discussions and presentation of meeting summaries to the joint group and to our hosts.

Copies of the presentations, papers and administrative information were distributed at the end of the meeting to all participants and may be obtained from the Scientific Secretaries on request. The full meeting report as a working document is also available on request from the Scientific Secretaries.

3. DISCUSSIONS AND RESULTS ACHIEVED

During the meeting, our discussions identified several areas, both technical and administrative, needing attention to effectively develop improved cold and directionally focused moderators. The areas identified include:

- Improved cross section libraries for neutron transport relevant to cold neutron sources
- Improved code physics to treat directionally enhanced moderators as well as cold moderators
- Improved reliability of access to codes for design and optimization of neutron sources
- Improved documentation of existing tools, data, and experience

3.1.Cross Section Libraries

Currently available cross section libraries relevant to cold neutron source analysis are inadequate. These libraries do not cover enough moderator materials, the materials they include are generally only covered at a single temperature in the un-irradiated state, and the accuracy of the kernels that are in the library is uncertain at best. Additionally, these libraries include very few structural and neutron-beam window materials. The libraries have been produced by different groups around the world, and must be obtained in different ways. Many of them have been demonstrated to be inappropriate for use in cold moderator development, and yet are still widely distributed, while others that have been demonstrated to work well have no formal distribution mechanism. We have tasked Mr Michal Mocko (USA) with the preparation of a report on those scattering kernels available, how to get them, and whatever validation may be available. We recommend that the IAEA in a more centralized way (e.g., through its Nuclear Data Section) consider setting up a website-based database and/or wiki for sharing scattering kernels, validation experience, etc.

The inconsistent manner in which scattering kernels are produced, distributed, and used frequently leads to significant ambiguity regarding which of several scattering kernels describing a particular material was actually used in a given calculation. We have tasked Mr Stuart Ansell (UK) with the development of a utility which extracts a signature from an ACE-formatted scattering kernel as represented in an XSDIR file and provides that signature for citation/documentation purposes. Eventually we hope to see such signature capability implemented directly in the relevant transport codes.

ACE-formatted cross section libraries do not have a mechanism for including single-crystal materials or macroscopic materials (e.g., such as the nano-crystalline diamond under exploration at the ILL, France), which are fundamental to the concept of the directed moderator. In more general terms, we question whether the current representation of scattering kernels in forms used by the transport codes are adequate for the calculations we now seek to perform; most specifically, the scattering kernels represent outgoing scattering as a series of (non-physical) discrete energies. This representation may be adequate for macroscopic calculations involving many collisions, and for systems with weak angular dependence, but causes problems in situations involving neutron beams and directionally enhanced moderators. The equivalent problem has already been addressed in the energy dimension, but this resulted in quite significant increases in kernel data storage requirements. The same treatment applied to angle would result in data storage requirements of several hundred megabytes per material, per temperature, etc. This does not seem tenable. We note that similar discussions regarding scattering kernel representations are currently active in the reactor physics community. We have tasked Mr Franz Gallmeier (USA) with approaching Michael Dunn (USA), from that community, to explore this overlapping interest, and we recommend that the IAEA commission another consultancy to convene data evaluators, data contributors, code developers, and users of scattering kernels, to recommend/implement changes in scattering kernel representation, library coverage, and code physics to satisfactorily treat the needs of both communities.

Improving the inadequate coverage of current cross section libraries will require new data. Many new materials will require detailed measurements of inelastic scattering, total cross section, powder diffraction, QENS, SANS, and reflectometry, all dependent on temperature, pressure, preparation method, annealing history, and irradiation history. Many otherwise well-known materials must be characterized with measurements specific to the macroscopic form of the component – for example, a neutron beam window made of aluminum will typically be a fairly highly textured piece of a specific alloy. A scattering kernel specific to an idealized poly-crystalline (powder) elemental aluminum does not well reproduce the effective transmission cross section of the beam window in use.

Many of these measurements are relatively straightforward, and can be performed (by adequately experienced researchers) at quite modest neutron sources. Such modest requirements represent an ideal avenue for involvement of researchers and facilities from developing countries and educational institutions. Ideally, this involvement would result in four major benefits: the data necessary for library development, the training of users/researchers in established standard measurement techniques, enhanced activity at otherwise under-utilized small sources at facilities in developing countries, and perhaps new instruments at these smaller facilities. In all cases, whether at small facilities with students or large facilities with experts, these measurements should always be base-lined to 300-K water. We have tasked Mr Lazslo Rosta (Hungary) to explore and coordinate this activity.

At the same time, some of the required measurements, for example inelastic scattering functions, require more sophisticated instrumentation and methods, and will need to be done at the larger facilities. Both FRM2 (Germany) and the ILL (France) have specific instrument development programs intended to support such activity. We would anticipate significant benefit to a broad “mapping” program of measurements at smaller facilities leading to selected candidate materials being proposed for detailed characterization with the formal user programs at large facilities and for prototypic moderator characterization at dedicated facilities like Hokkaido and LENS. Mr Emmanuel Farhi (France) has volunteered to coordinate proposals to these large scattering facilities.

Once the data necessary for generating a neutron scattering kernel are available, it is by no means a simple process to produce a useable kernel. Currently available tools are difficult to use, and there are few experts in the generation of scattering kernels even from complete information. We have tasked Mr Guenter Muhrer (USA) and Mr Franz Gallmeier (USA) with the development of a script/wrapper for the various codes available to produce scattering kernels given either analytically provided (e.g., AbInit / Aclimax) or experimentally provided data.

We also note that a big number of potential materials for advanced cold moderators have been characterized by inelastic neutron scattering for reasons having nothing to do with their potential use as moderators. The data taken in such measurements provide yet an unexplored opportunity. Upon the development of a simple figure-of-merit for neutron moderation, it would be in principle a relatively straightforward task to automate a search through the archives of the larger neutron scattering facilities to identify materials worthy of study as advanced neutron moderators – materials which otherwise might not have been considered. In addition to the technical aspects associated with such a survey, this activity would require access to the data. Different facilities have different policies for public access to neutron scattering data. We have tasked Mr Peter Willendrup (Denmark) with identifying the relevant data access policies. Mr Stuart Ansell (UK) has volunteered to develop a data-mining framework to search through inelastic scattering data sets, applying the scripts described above (i.e., to be developed by Muhrer and Gallmeier) to provide a figure-of-merit for each candidate data set / material.

3.2. Code Physics

As described above, currently available scattering kernel representations do not provide satisfactory (or in some cases any) representation of essential physics processes. This shortcoming is mirrored in the neutron transport codes – these physics processes are simply not implemented. Eventually, a transport code system used to model a neutron source and its beamlines should include neutron reflection, refraction, crystalline diffraction, small-angle scattering, polarization, gravity, magnetic fields, single crystals, and better treatment of real thermal scattering. While we note reflection and refraction have recently been implemented in development versions of MCNPX (USA), and PHITS (Japan) includes magnetic effects, SANS, and gravity, no single transport code includes all these physics processes. Additionally, the desire to correctly model the perturbations on a reactor core from the inclusion of neutron beam tubes (necessary to best predict both neutron beam characteristics and reactor performance) implies the need for the code to treat criticality. We exhort our participants to encourage developers of the various codes to implement these physics processes in their codes, both the standard codes such as MCNPX and PHITS and other relevant transport codes such as Fluka and Geant (both Europe), which may become more desirable as access restrictions associated with MCNPX become more onerous. One additional option suggested by the group was that developers of transport codes are encouraged to provide a more complete, more effective, and better documented "plug-in" architecture for the addition of new physics; in this way we as a community can better leverage specific developments needed and made by individual members. We have tasked Mr Guenter Muhrer (USA) with the preparation of a report covering code physics and capabilities, including what physics is treated in which codes.

3.3. Code Access

Access to the codes used in the analysis, design, and optimization of neutron sources are frequently restricted by various laws and regulations. Such restriction is understandable, given the applicability of these codes to many aspects of neutron and general radiation transport, not just to the development of neutron source facilities for research purposes. However, restrictions on access to these codes, and even more sudden and unpredictable changes in access requirements to these codes, make ongoing research projects very difficult. There are several codes used world-wide for different aspects of (slow) neutron source design, but the most common are MCNP, its high-energy multi-particle variant MCNPX, and PHITS. Access to the MCNP and MCNPX codes is governed by the United States Department of Energy (although such authority was recently shifted to the Department of Commerce for a short time before being returned to the DOE), and access requirements change so frequently that some researchers who were formerly on the code development team(s) are now not allowed to access the code they themselves contributed. Additionally, these codes are frequently specifically required for the analysis of some safety aspects of nuclear facilities by national safety organizations, even though the changing code access requirements sometimes preclude their use by facility personnel. This situation is untenable; so much so that we as individuals and as a community have some difficulty considering the use of MCNP and/or MCNPX as a viable ongoing proposition. We note that, because the newest version of PHITS incorporates parts of MCNPX, it might become subject to the same constraints. As indicated above, we have tasked Mr Guenter Muhrer (USA) with the preparation of a report covering code physics and capabilities, as well as access requirements.

We also note that effective access to the code does not simply involve being able to get the code – but also to being able to use the code. This is especially a problem for smaller facilities, and at developing countries, where, in many cases, there are no qualified individuals available. It would be highly desirable to implement/regularize some sort of education and training programs for neutron source modeling. There are multiple mechanisms by which such programs might be implemented. The developers of a given code will frequently sponsor training sessions or courses on their code; for example there will be a McStas training session in November 2011, in association with a neutron scattering meeting in Japan. It is recommended that the IAEA provides support for the participants from the developing countries to attend. The IAEA, together with UNESCO, further sponsor the International Centre for Theoretical Physics (ICTP or popularly known as the Trieste school), which brings students from developing countries together for one-week or even longer courses. While the program for 2011 is already completely booked, it might be possible to implement such a course in the coming years.

3.4. Documentation

One aspect of documentation that is frequently held forth as desirable is some sort of survey picture of different facility/moderator brightness numbers. It should contain data from all neutron facilities world-wide. ESS apparently has plans to collect this information and make it available to the community. Mr Ferenc Mezei (ESS) will draft a data template for what should be included in such a report, involving someone from the research reactor community to make sure that the template adequately samples / describes research reactor sources as well. The IAEA is asked to assist in collecting such a data through the existing contacts in different Member States.

Additionally, we see great advantage to a dedicated cold source benchmarking activity, perhaps along the same lines as the spallation benchmarking activity recently coordinated by the IAEA. We recommend the development of such a benchmarking activity.

4. CONCLUSIONS AND RECOMMENDATIONS

In the concluding session the meeting participants formulated the following specific recommendations to the IAEA:

1. **Initiate and coordinate flux/brightness comparisons of different cold neutron sources**, both research reactor and neutron spallation based
2. **Initiate and coordinate a scattering kernel database/download site**, covering moderating materials, window materials, structural materials, and nano-particulate materials, including a full range of temperatures down to those appropriate for Very Cold Neutron source design, and eventually covering varying levels of radiation damage. This website should also serve as a repository/distribution mechanism for various utilities dealing with scattering kernel production and use
3. Through its own pathways and via its Member States, **provide statements and encouragement to maintain accessibility, and regularity of accessibility, to standard transport codes used for design, analysis, and safety qualification of cold sources, neutron source facilities**, etc. Such codes include MCNP, MCNPX, PHITS, etc.
4. **Organize a dedicated consultancy to convene data evaluators, data contributors, code developers, and users of scattering kernels.** This consultancy should consider not just what materials are covered, but also the manner of expression – for example the current S(a,b) format implementation from NJOY, if taken to sufficient energy/angle detail, requires several hundred megabytes for a single temperature of a single material.
5. **Initiate, support and coordinate a cold and/or advanced moderator benchmarking activity**

6. **Initiate and support a new Coordinated Research Project** on Advanced Moderators to Enhance Cold Neutron Beam Production for Materials Research and Applications (tentative title). The following preliminary structure is proposed for this new CRP

    - Goals
        - improve the utilization / productivity of neutron sources / facilities by enhancing neutron beam intensities
        - provide access to more end users
    - Topical Focus
        - Materials for advanced moderators
        - Computer codes: access and capabilities
        - Scattering kernels: assessment, availability, documentation, and production
        - Reports of ongoing prototype moderator implementations
    - Desired Outcomes
        - Increased user throughput
            - Perform more experiments
            - Enable harder experiments
        - Enhance facility performance
        - Extend neutron scattering, etc., to additional, smaller facilities
        - Enable additional technological / material advances
    - Desired Output
        - Reports describing existing kernels, methods, and facilities
        - Database of kernels / access to same
        - Sets of codes / utilities
        - Completion of experiments
            - Benchmark / validation
            - New concepts
        - Establish / strengthen / formalize current community of cold source developers, etc.

ANNEX I. WORKPLAN FOR THE NEXT 12 MONTHS*

Action	Deadline	Coordination
Prepare data template for submission of facility /advanced moderator performance data to centralized repository for collection and documentation	Q2 2011	Mr Mezei
Work with research reactor community to identify needs in scattering kernel representation, treatment, and libraries	Q2 2011	Mr Gallmeier
Develop and distribute a utility for extracting a scattering kernel “signature” for documenting exactly which kernel is represented in a specific ACE-formatted file or transport calculation.	Q2 2011	Mr Ansel
Identify access restrictions to existing neutron scattering data to facilitate data-mining for candidate advanced moderator materials	Q2 2011	Mr Willendrup
Prepare report listing and describing the scattering kernels available for cold moderator materials, structural materials, and neutron beam window materials, their availability, and their validation / usage.	Q3 2011	Mr Mocko
Organize a dedicated consultancy to convene data evaluators, data contributors, code developers, and users of scattering kernels.	Q3 2011	IAEA
Explore the potential to perform dedicated nuclear data measurements at medium power research reactors and developing countries in particular	Q3 2011	Mr Rosta
As a result of the above CM, implement a website-based scattering kernel list, repository / distribution site, and documentation collection.	Q4 2011	IAEA
Develop script / wrapper to produce scattering kernel library from either analytical tools (i.e., AbInit / Aclimax) or measured inelastic scattering data.	Q4 2011	Mr Muhrer & Mr Gallmeier
Develop data-mining framework for searching existing inelastic scattering datasets to identify candidate advanced moderator materials.	Q4 2011	Mr Ansell
Prepare report describing neutron transport codes relevant to cold neutron source design, including code physics, usage, features, and access restrictions	Q4 2011	Mr Muhrer

* In addition to the meeting conclusions and recommendations (see section 4).

ANNEX II. MEETING AGENDA

Consultancy Meeting on
Directionally Focused Moderators for Enhanced Neutron Beam Intensities to Support Materials Research and Applications

Monday December 06, 2010

CRP sessions dedicated to Micro-Focusing SANS and Transmission Measurements

Location: Room F0814

08:00 – 09:00	Registration
09:00 – 10:00	Opening of the Meeting *Welcome Remarks* *Announcements* *Election of Chairperson:* ***Mr M. Furusaka*** *Election of Rapporteur:* ***Mr D. Baxter*** *Discussion and approval of the Agenda* *Administrative arrangements for the meeting*
09:30 – 09:45	Status Report on the CRP Purpose of a final RCM *Ms F. Mulhauser, IAEA*
09:45 – 10:15	*Coffee break*
10:15 – 12:00	Progress Report (2×40minutes) and Discussions **Session: Micro focusing SANS** ***Malaysia*** *(Mr A. Mohamed)* ***Indonesia*** *(Mr E. Putra)*
12:00 – 13:30	*Lunch Break*
13:30 – 15:00	Progress Report (2×40minutes) and Discussions **Session: Micro focusing SANS** ***Japan*** *(Mr M. Furusaka)* ***Czech Republic*** *(Mr P. Mikula)*
15:10 – 15:30	*Coffee break*
15:30 – 17:00	Presentations (2×40minutes) and Discussions **Session: Transmission measurements** ***Argentina*** *(Mr R. Granada for Mr Santisteban)* ***Japan*** *(Mr Y. Kiyanagi)*
17:00 – 17:30	Discussions: Outputs and success

Tuesday December 07, 2010

Joint Sessions on Cold Neutron Sources: Morning dedicated to CRP, Afternoon to CS

Location: Room A2311

08:30 – 09:10	Presentations of participants Presentations of plans for the two meetings Mr D. Ridikas and Ms F. Mulhauser *Election of Chairperson:* ***Mr Y. Kiyanagi*** *Election of Rapporteur:* ***Mr E. Iverson***
09:10 – 13:00	CRP Presentations (5×40minutes) and Discussions **Session: *Neutron sources***

	Argentina *(Mr R. Granada)*
	India *(Mr S. Baisu)*
	Japan *(Mr F. Hiraga)*
	Russia *(Mr E. Shabalin)*
	Russia *(Mr S. Kulikov) (20 minutes)*
	USA *(Mr D. Baxter)*
13:00 – 14:00	*Lunch Break*
14:00 – 18:50	CS Presentations (6×30minutes) and Discussions
	USA-UK*; SNS/LENS/ISIS (Mr Iverson)*
	UK-USA; ISIS/SNS (Messrs ***Ansell*** *&* ***Gallmeier****)*
	Hungary, BNC (Messrs ***Rosta****,* ***Grósz*** *&* ***Füzi****)*
	OPAL/ANSTO*, Australia (Mr Braoudakis)*
	FRM-II/TUM*, Germany (Mr Roehrmoser)*
	ILL*, France (Mr Farhi)*

Wednesday December 08, 2010

Joint Sessions

Location: Room F0814

08:30 – 13:00	CS Presentations (6×30minutes) and Discussions
	LANL, USA (Messrs ***Mocko*** *and* ***Muhrer****)*
	ATI*, Austria (Mr Rauch)*
	ESS*, Sweden (Mr Mezei)*
	PNPI*, Russia (Mr Mityukhlyaev)*
	JPARC*, Japan (Mr Maekawa)*
	PSI*, Switzerland (Mr Wagner)*
13:00 – 14:00	*Lunch Break*

Joint Sessions

Location: Room A2311

14:00 – 18:00	Discussions about collaborations and objectives of both meetings
18:30 – 19:30	Hospitality Events

Thursday December 09, 2010

Separated Sessions

Location: Room A2311 and Room F0814

09.00 – 13:00	Discussions and drafting of the meeting report
13:00 – 14:00	*Lunch break*

Joint Sessions

Location: Room A2311

14:00 – 15:00	Final Discussions and adoption of the meeting reports
15:00 – 15:30	Closing of the meeting

ANNEX III. LIST OF PARTICIPANTS

Consultancy Meeting on Directionally Focused Moderators for Enhanced Neutron Beam Intensities to Support Materials Research and Applications

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