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Summary Report of the Consultants' Meeting on

Compilation of Thermal Neutron Scattering Data for Experimental Nuclear Reaction Data Library (EXFOR)

IAEA Headquarters, Vienna, Austria

2 - 4 November 2015

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April 2016

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ABSTRACT

The Consultants' Meeting on "Experimental Nuclear Reaction Data (EXFOR) Compilation of Thermal Neutron Scattering Data" was held at the IAEA Headquarters in Vienna from 2 to 4 November 2015. The evaluation and experimental methodologies applied at thermal neutron energies, including: the total and differential cross section measurements, the data analysis and the theoretical methods were discussed during the meeting. The participants have agreed on recommendations on the data reporting for EXFOR and drew up guidelines for the compilation of the thermal scattering experiments. Summaries of the presentations, discussions and recommendations are reported here. The presentations given at the meeting are available on https://www-nds.iaea.org/index-meeting-crp/CM-THSC-2015/ .

April 2016

TABLE OF CONTENTS

1. Introduction

A consultants' meeting on "Experimental Nuclear Reaction Data (EXFOR) Compilation of Thermal Neutron Scattering Data" was held at IAEA Headquarters, Vienna, Austria from 2- 4 November 2015. Six participants: Florencia Cantargi, David V. Baxter, Li (Emily) Liu, Emmanuel Farhi, Yoshiaki Kiyanagi, and Jose Ignacio Marquez Damian have attended this meeting. IAEA was represented by N. Otsuka, V. Semkova and S. Simakov. The list of participants and their affiliations are summarised in Appendix IV.

The Meeting was organized following the recommendations of the 30th Meeting of the International Nuclear Data Committee to collect the results from experiments related to thermal scattering law (TSL) data development and make them available from the EXFOR database.

In the welcome address A. Koning, Section Head of the Nuclear Data Section, greeted the participants and stated that the completeness and the consistency of the EXFOR compilations are essential for the proper analysis and evaluation of the experimental nuclear reaction data. In this respect the review of the status of the thermal scattering data in EXFOR is timely, considering the task of the new Subgroup 42 of the OECD-NEA Working Party on International Evaluation Cooperation of the Nuclear Science Committee to revise and extend the TSL data.

The participants elected E. Farhi as a Chairperson of the meeting and J. I. Marquez Damian as a Rapporteur. The agenda was discussed and adopted (see Appendix III).

During three days participants gave presentations (available on https://www-nds.iaea.org/index-meeting-crp/CM-THSC-2015/) and had intensive discussions. The total and differential cross section measurements performed at different experimental facilities were presented. A summary of the experimental and theoretical methodologies applied to obtain the scattering law data was given by E. Farhi. The participants discussed experimental data needs for the thermal scattering library evaluations, the status and the compilation rules of thermal neutron data in EXFOR. The discussions resulted in: update of the thermal-neutron scattering part of the compiler's manual (LEXFOR); adoption of a template with essential information to be compiled for a time-of-flight thermal measurement (Appendixes II); list of materials of interest for nuclear research and applications; consolidated conclusions and recommendations (see following Sections). It was pointed out that, in addition to the differential and total cross sections compiled in EXFOR, a collection of derived or complementary data, such as phonon spectra; structural parameters; thermal neutron scattering kernels etc., in a dedicated section of EXFOR or in a separate repository will provide information that will facilitate further developments in thermal neutron scattering studies and applications

The Nuclear Data Section acknowledged all participants for their cooperation and contribution to this Meeting.

2. Presentation summaries

2.1 V. Semkova, IAEA-NDS: "Objectives of the Meeting"

Thermal neutron scattering cross section data are important in many fields of science and applications. The thermal data are needed for neutronics calculations of the various reactor and benchmarks assemblies. Low temperature measurements can also determine the effect of the crystal lattice and improve the knowledge of the resonance parameters. Such data are essential for cold moderator applications. Neutron monochromators and filters are based on coherent scattering or resonance absorption in certain materials. Thermal scattering data for organics are needed for neutron dosimetry and medical applications.

Recently there has been a renewed interest in revisiting and extending the existing thermal neutron scattering libraries. Completeness and consistency in the compilation of thermal neutron induced data in EXFOR database will contribute to and facilitate the new evaluations.

Scattering of slow neutrons depends not only on the sample composition but also on the atomic structure and dynamics, because the wavelength of slow neutrons is of the order of inter atomic distances and the energy is comparable to the energy of bonding and thermal motion of the atoms. The directly measured quantities as a function of the neutron momentum and energy transfer are further processed applying various concepts and approximation. The evaluated data in the thermal neutron libraries are expressed in terms of thermal scattering kernels. In this respect the main objective of the meeting is to discuss what type of data and additional information needs to be compiled in EXFOR. Recommendations and guidelines for the compilation of the thermal neutron data will ensure that the experimental details needed for the proper data evaluations are provided.

Although the thermal scattering is included in the scope of the EXFOR compilations the database cannot be considered as complete and probably the compilation rules need to be reviewed and updated. Many scattering data exist in the scientific literature. However, some of them have been measured for material science studies or other applications. So, not all of them are relevant to nuclear research and applications. A list of materials needed for nuclear evaluations will help EXFOR community in defining the compilation priorities.

2.2 Naohiko Otsuka, IAEA-NDS: "Basic Questions on Compilation of Experimental Thermal Neutron Scattering Data"

EXFOR compilers do not have many opportunities to draw special attention to compilation of the thermal neutron scattering data. Apart from its temperature dependence, it is "legal" to compile many quantities (*e.g.*, total cross section) as those above the thermal energy region from the view of the official EXFOR format rule. There are some codes specific for the thermal neutron scattering data (*e.g.*, `COH` for coherent scattering, `INC` for incoherent scattering, `BA` for bound atom, `FA` for free atom). We do not often meet new articles related to these codes, but the compiler's manual (LEXFOR) must be improved so that we may do necessary revisions appropriately when necessary (*e.g.*, improvement of consistency within EXFOR entries). The paper summarizes a brief statistics of EXFOR for thermal neutron scattering data, and also introduces two questions in order to improve the EXFOR dictionary and compiler's manual.

1. Statistics of the EXFOR library for thermal neutron scattering data

In order to obtain a brief statistics of thermal neutron scattering data in EXFOR, I searched for EXFOR by the following criterion:

- Projectile: `N` (neutron)
- Quantity: `CS` (cross section), `DA` (angular differential cross section), `DAE` (double differential cross section) or `L` (scattering length)
- Incident energy: less than 0.01 eV.

Then I found 811 cross section data sets, 2 angular differential cross section data sets, 1 double differential cross section data sets, and 289 scattering length data sets. It shows that we have very few data sets for differential data in EXFOR though they are also powerful to validate $S(\mathbf{q},\omega)$. In order to examine the completeness of EXFOR for the past experiments, I checked EXFOR against the experimental works cited for evaluation of H_2O, D_2O, ZrH_x and graphite data by Mattes and Keinert (Uni. Stuttgart) [1]. The result summarized in **Table 1** implies that we still miss many experimental works in EXFOR.

2. Questions on terminology and coding rule

a) Scattering amplitude and scattering length

There are many data tagged by the quantity code `AMP` which is expanded as "scattering amplitude" in the EXFOR dictionary. In my observation, many EXFOR data sets compiled with `AMP` are introduced as the scattering *length* in the source articles. For elastic scattering, the low energy limit of the scattering amplitude is equal to the scattering length but with the opposite sign. Among 100 AMP

values compiled in EXFOR, about 30 AMP values are negative, and they are for neutron scattering with hydrogen (10 values); neutron (5 values); lithium (3 values); vanadium (2 values), most of which are also negative in various tabulation [*e.g.*, 2,3] of scattering *lengths*. Clarification of the actual definition of the code AMP would be desirable for both EXFOR compilers and users.

Table 1. Availability of exp. data cited by Mattes et al. [1] evaluation in EXFOR (N/A: not available).

Material	Reaction	Quantity	Author	Reference	Lab.	EXFOR #
H_2O	SCT	DAE	F. Bischoff+	R,RPI-328-87,1967		**N/A**
	SCT	DAE	J.R. Beyster	J.NSE,31,254,1968	1USAGA	11029
	TOT	CS	J.L. Russell+	R,GA-7581,1966	1USAGA	11162
	TOT	CS	K. Heinloth	J,ZP,163,218,1961	2GERMUN	21341
	TOT	CS	K.N. Zaitsev+	J,SJA,70,238,1991		**N/A**
	TOT	CS	M. Dritsa+	R,EANDC(OR)-63,1967	2GRCATH	20176
	TOT	CS	S.B. Herdade+	P,INDC(BZL)-2-22,1969	3BZLIPE	30229
ZrHx	SCT	DAE	F. Bischoff+	R,RPI-328,1966		**N/A**
	SCT	DAE	S.N. Purohit+	C,67ANNARB,1,407,1967		**N/A**
	SCT	DA	G.W. Carriveau	R,GA-8345,1967		**N/A**
	SCT	DA	S. Kornbichler	J,NK,7,281,1965		**N/A**
	SCT	CS	W.L. Whittemore	R,GA-5554,1964		**N/A**
	SCT	CS	U. Schmidt	ATKE,12,385,1967		?
	SCT	CS	W.L. Whittemore	R,GA-4490,1958		**N/A**
D_2O	SCT	DA	S. Kornbichler	J,NK,7,281,1965		**N/A**
	SCT	DA	T. Springer	J,NK,6,87,1964		**N/A**
	TOT	CS	F. Kropff+	W,KROPFF,1974	3ARGCAB	30283
	TOT	CS	V.W. Meyers	W,MEYERS,1953	1USABNL	11019
	TOT	CS	L.J. Rainwater+	J,PR,73,733,1948	1USACOL	11145
	TOT	CS	S. Dritsa+	W,DRITSA,1971	2GRCATH	20038
Graphite	SCT	DAE	W.L. Whittemore+	J,NSE,33,31,1968		**N/A**
	TOT	CS	A. Steyerl+	J,ZP,267,379,1974	2GERMUN	21016
	TOT	CS	J.M. Neill+	R,GA-6753,1965		**N/A**
	TOT	CS	D.J. Hughes+	R,BNL-325,1958		?
	TOT	CS	L.S. Kothari+	J,PR,106,230,1957		**N/A**

b) Incident neutron energy dependent scattering length?

Because the scattering length is related with the scattering amplitude at zero energy limit, it seems redundant to compile scattering lengths (or the cross section related with the scattering length by $\sigma=4\pi b^2$) with its incident energy. Koester also often introduces this cross section as σ_0 (cross section at zero energy, e.g.[4]). However, the current EXFOR system requires the incident neutron energy as the independent variable of the scattering length, and we often see AMP data sets (or the cross section data sets derived from the scattering length by the formula) with finite neutron energies. Even though the experimentalists use neutron beams at specific energies to obtain these quantities, probably it is not their intentions to report these quantities at the specific energies. It would be better to consider whether we really need to specify incident energy for these quantities.

References:
[1] M. Mattes and J. Keinert, INDC(NDS)-0470 and 475, 2005.
[2] H. Rauch and W. Waschkowski, "Neutron scattering length", in Neutron Data Booklet, ILL, 2003.
[3] L. Koester, H. Rauch, E. Seymann, Atom. Data Nucl. Data Tables **49** (1991)65.
[4] L. Koester, W. Waschkowski, J. Meier, Z. Phys. A**337** (1990)341.

2.3. D.V. Baxter, Indiana University: "Compact Accelerator-driven Neutron Sources as tools for nuclear data"

It is well recognized by those using simulation codes for the design of nuclear systems other than nuclear reactors that the existing data libraries are inadequate for many purposes. This comes primarily from the lack of relevant data for materials and/or conditions of interest, but also from the lack of fidelity of some existing data when applied to these "novel" situations. As nuclear technologies expand in their scope, such novel applications (such as design of small neutron sources, developing treatment plans for neutron and proton radiotherapy, etc.) will become more common and the need for adequate data on new materials can therefore be expected to expand over the next few decades. Unfortunately, the acquisition of the primary neutron scattering data that would be suitable for the construction of useful thermal nuclear data models is not generally given a high priority by the review committees that are typically responsible for allocating beam time at the major neutron scattering facilities throughout the world. It is our position at LENS that this is an area where smaller neutron sources may be able to provide important contributions.

LENS is a compact Accelerator-driven Neutron Source (CANS) that has been operating for a little more than one decade at Indiana University. At LENS we have demonstrated the ability to measure neutron transmission through liquids over an energy range from less than 0.1 meV to 1 eV and a temperature range from roughly 10^{o}C to 70^{o}C with a single accelerator operational setting with roughly 1 day of beam time per measurement. These ranges (of both energy and temperature) could be extended if a need to do so arises (albeit with possibly longer data acquisition times). Although not by itself a sufficient validation for any proposed model data set, such total cross section measurements should be seen as a convenient and necessary first step in any such validation process. Most CANS facilities would be able to provide similar capabilities, and therefore such facilities should be viewed as an important potential resource in the validation of nuclear data.

At LENS in particular, it is also possible to provide additional integral data against which models of certain materials (particularly those of interest in neutron moderator applications) can be tested. Thanks to materials choices made for the design and construction of LENS, it is possible to have relatively direct access to the neutron target shortly after the proton beam has been shut down [1]. This allows experimental studies on novel moderator materials and designs (measurements that include not only the emitted spectrum, but also the emission time distribution at up 7 energies over the range from 2.8 meV to 135 meV). We are in the middle of a series of benchmark tests of this capability at LENS using water moderators of various thicknesses, and we soon expect to start similar measurements on other materials of interest. We wish to also point out that in some of the studies that we have performed so far have involved test geometries that include design elements that are single crystals, and we have considered situations in which neutron refraction may play a significant role. We also recognize that in some other neutron applications these effects (single crystal scattering and refraction) can also be important (e.g. monochromators or filters in neutron scattering instruments and ultra-cold neutron transport). In recognition of this, recent work has been devoted to incorporating refractive and single crystal effects into traditional neutron transport codes MCNP [2] and GEANT-4 [3]. The Nuclear Data Section should consider carefully whether EXFOR is a suitable venue for the storage of data relevant to single crystal effects.

References:
[1]. C. M. Lavelle et al., Nucl. Instr. Meth. **A 587**, 324-341 (2008).
[2]. F. X. Gallmeier, et al. submitted to Nucl. Inst. Meth.
[3]. X-X Cai, ``GEANT-4 extensions for neutron scattering in crystalline materials", presented at ECNS 2015.

2.4 Li (Emily) Liu, Rensselaer Polytechnic Institute: "Thermal Neutron Scattering Measurements at Spallation Neutron Source and Analysis"

We have performed time of flight inelastic neutron scattering measurements of light water (H_2O), high-density polyethylene (CH_2), and quartz (SiO_2) at Fine-Resolution Fermi Chopper Spectrometer (SEQUOIA) and Wide Angular-Range Chopper Spectrometer (ARCS) of Spallation Neutron Source (SNS) in Oak Ridge National Laboratory. The experiments that have been done and analyzed are listed in Table 1.

Table 1. The time of flight inelastic neutron scattering measurements performed in SNS of ORNL.

Materials	**The instruments utilized in Spallation Neutron Source (SNS)**	
	Fine-Resolution Fermi Chopper Spectrometer (SEQUOIA)	**Wide Angular-Range Chopper Spectrometer (ARCS)**
Light Water (H_2O)	E_I: 55, 160, 250, 600, 1000, 3000, 5000 meV Ω: 3-58^o in 1^o increments Temp = 300 K	-
Polyethylene (CH_2)	E_I: 55, 160, 250, 600, 1000, 2000 meV Ω: 3-58^o in 1^o increments Temp = 300 K	E_I: 50, 100, 250, 700 meV Ω: 3-125^o in 1^o increments Temp = 5, 295 K
Quartz (SiO_2)	-	E_I: 50, 100, 250, 700 meV Ω: 3-125^o in 1^o increments Temp=20, 300, 550, 600 ^{o}C

The work was designed specifically to fit the nuclear data needs therefore various incident energies and various temperature data have been taken. More importantly, we carefully analyzed the experimental data to double differential cross section vs. angle and final energy and are in the progress of comparing and integrating the experimental data with various theoretical and simulation approaches. And we are in the process and progress to formulize the approach from Double Differential Cross Section (DDSCS) to S(Q, ω), Generalized Density Of States (GDOS), and S(α,β).

In Figs. 1 and 2, we show the process that we so far successfully took two routes:

1) Theory Norm in Fig. 1: DDSCS → S(Q, ω) → GDOS, then normalized according to Theoretically derived Vibrational Density of States (VDOS)→ NJOY2012 → MCNP → fit back to DDSCS.

2) Exp-Norm in Figs. 1 and 2: DDSCS → S(Q, ω) → Generalized Density Of States (GDOS), not normalized according to Theoretically derived Vibrational Density of States (BDOS)→ NJOY2012 → MCNP → fit back to DDSCS.

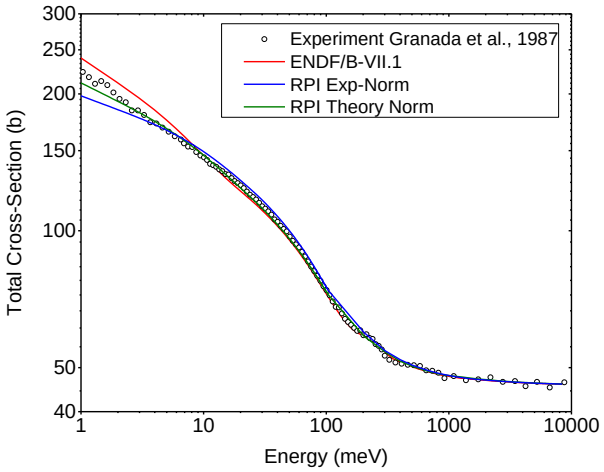

Fig. 1. GDOS derived from experimental DDSCS, with or without normalization with theoretical VDOS in comparison of total cross section provided by total scattering experiments.

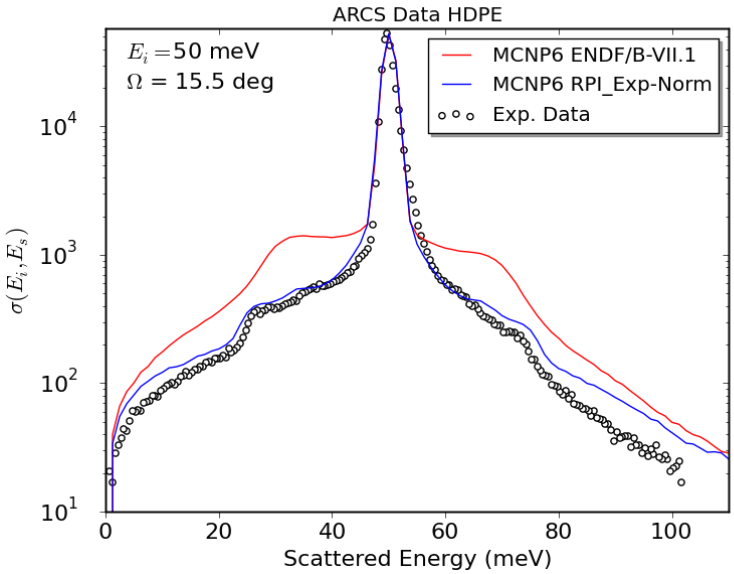

Fig. 2. Example of the GDOS derived from experimental DDSCS, without normalization with theoretical VDOS, can be utilized to derive DDSCS and it agrees well with direct experimental DDSCS, in comparison with MCNP6 calculation based on ENDF/B-VII.1.

So far we have observed the following:

- The thermal differential scattering experimental data, as the most accurate experimental data, can be used to generate phonon spectrum and the angular and energy range will then to maximized to serve the need to benchmark S(α,β) evaluations.
- The experimentally derived phonon spectrum is in good agreement with the total cross section measurement. Using experimentally derived phonon spectrum, the agreement between the MCNP-6 calculation and the experiment is improved. Normalizing the experimental phonon spectrum with theoretical phonon spectrum will improve the total cross section calculation, but cause more discrepancy when we transfer phonon spectrum back to DDSCS.

- Deriving phonon spectrum from double differential scattering experiment to get generalized density of states (GDOS) requires measurements at 5 K (clearer modes will be shown).
- Double differential scattering experiments and total scattering experiments are all needed to serve different purposes of the validating process of simulation or theory.

Acknowledgement:

- Key collaborators (Goran Arbanas, Luiz Leal, Mike Dunn).
- Special thanks to the help from scientists at SNS: Alexander Kolesnikov, Doug Abernathy, and Luke Daemen
- The project is funded by DOE NCSP.
- Research at Oak Ridge National Laboratory′s Spallation Neutron Source was supported by the Scientific User Facilities Division, Office of Basic Energy Sciences, U. S. Department of Energy.

2.5 F. Cantargi, Centro Atomico Bariloche: "Total Neutron Cross Section Measurement for Thermal Scattering Library Evaluation"

In this presentation the activities of the Neutron Physics Department at Centro Atómico Bariloche (Argentina) are described. The group activities started in 1970 towards a small pulsed neutron source, a 25 MeV eLINAC. For more than 40 years the group has been working on neutron physics and applications to condensed matter research, materials science and nuclear engineering [1].

The thermal scattering nuclear data subgroup is integrated by 3 people: Rolando Granada who mostly work in scattering theory and neutron sources, Ignacio Márquez who works in developing scattering kernels for materials of nuclear reactor applications and benchmarking and Florencia Cantargi who works on the developing of scattering kernels for other materials with no direct application in nuclear reactors such as cold moderators or neutron filters.

Throughout these years the group was involved in the development of many cross section libraries which were demanded not only by people working at the same institution, also from different parts of the world. The working methodology was described. It consists on developing the scattering kernel to produce a total cross section and, to compare to a measured one, as a first step in validation. Then, as a second step in validation, this cross section library is used in a calculation of other magnitude (neutron spectrum for example). Measurements can be done at the eLINAC by applying the transmission and time-of-flight techniques. If no sample is available, data from EXFOR or from bibliography are used to compare to the models. We are aware that the total cross section is not the only magnitude that should be used for comparing but it is the first requirement it has to be fulfilled.

Although a low intensity pulsed neutron source is clearly not competitive with an accelerator orders of magnitude more intense, for most of the possible applications, it is nevertheless very useful to test ideas and the ensuing methods born from the successful ones. This is particularly true for total cross section measurements. At present, the eLINAC is stopped due to technical problems in the electron source but it is being renovated as part of a project to support neutron sciences for the upcoming RA-10 reactor.

Three examples of measurements and calculations were shown. The first was the measurement of Mylar in 1972 which produced the first publication of the group. The second one was mesitylene which is a cold moderator material which has deeply been studied in the group as part of a collaboration with people from the Frank Laboratory of Neutron Physics (Joint Institute for Nuclear Research) in Dubna, Russia who used this cross section library in the design of the cold neutron source of the IBR-2M reactor which is at present operative. Measurements and calculations were shown.

The last example was a single crystal sapphire which was studied as a neutron filter. It was emphasized that measurements and calculations were done taking into account that the studied material was a perfect single crystal and that measurements were performed with the neutron beam in the same direction of the main axes of the crystal. This led to the question: Do we need to store incident angles for total cross sections? We all agreed on that need. In such cases it is important to make clear that measurements were done with a specific orientation of the sample. This should be included in some way in the existent TOF-template.

References:

[1] *http://www2.cab.cnea.gov.ar/~nyr/tsl_eng.html*

2.6 J.I. Marquez Damian, Centro Atomico Bariloche: "Experimental Data Needs for Thermal Scattering Library Evaluation"

If we consider the problem of obtaining neutron scattering libraries by the process of evaluation (i.e. the application of models to the production of an evaluated nuclear data library, as opposed to the direct use of experimental results), experimental data plays several roles which have to be considered for the inclusion in EXFOR.

Methodologies for the evaluation are summarized in the diagram shown in Fig. 1. The evaluation can be performed:

i) in a traditional way, where a set of models is fed with selected input parameters, either obtained by experimental or theoretical methods [1, 2, 3, 4];

ii) by the calculation of such parameters using computational chemistry methods (molecular dynamics, density functional theory), [5, 6, 7], or

iii) by direct calculation from computational chemistry results[1] [8, 9, 10].

[1] The work presented in reference [9] only enters this definition of evaluated nuclear data in part, because it combines experimental and numerical results.

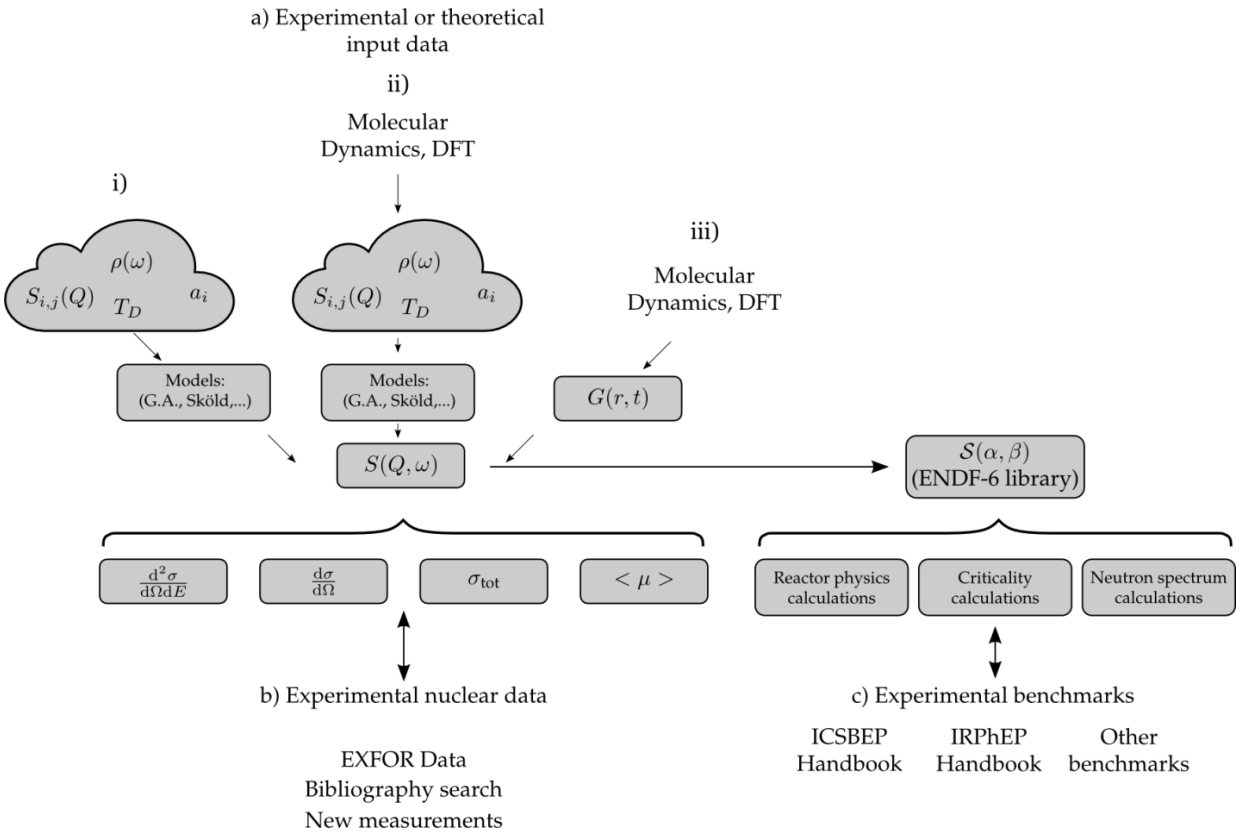

Fig. 1: Review of evaluation methodologies.

All three methodologies converge to the calculation of the dynamic structure factor, S(Q,ω), from which observable neutron scattering quantities can be calculated:

- Double differential scattering cross sections ($d^2\sigma/dE'd\Omega$),
- Angular differential scattering cross section ($d\sigma/d\theta$),
- Total scattering cross sections,
- Neutron diffusion parameters.

The dynamic structure factor can be stored in standard form and used to compute nuclear data libraries for transport calculation codes. These codes can be utilized to simulate benchmark systems for benchmarking.

Therefore, in this framework we have experimental data as:

a) Input parameters,

b) Derived neutron scattering quantities, and

c) Experimental benchmark results.

For any of these categories data can be compiled and distributed but, in my opinion as an evaluator, I expect EXFOR to provide the data described in b) for validation, and eventually part of the input parameters described in a), as long as they can be considered experimental neutron scattering data. The data described in c) is usually too complex to be stored in EXFOR and might be the subject of other efforts such as ICSBEP, IRPhEP, SINBAD, etc. because it needs the definition and evaluation of experimental benchmark problems, which requires the specification of the geometry, conditions, boundary conditions and sources in the problem.

In a nutshell, I recommend the incorporation of double differential, differential (in angle and energy) and total scattering cross sections, and neutron diffusion parameters. The reasons for this are:

- Nuclear data should be "model agnostic": frequency spectra are needed for TSL evaluation, but only when the Gaussian approximation is used. Perhaps we can make a database to help evaluators, but it is not strictly nuclear data.
- Nuclear data should be a physical property: neutron spectrum is a property of the material only in ideal conditions; in reality, you need to model the system (a benchmark model).
- Nuclear data should be as close as possible to the measurable quantity: the angular differential cross section $d\sigma/d\theta$ is nuclear interaction data, the structure factor S(Q) is not.

Based on this, my recommendations are:

Recommendation I:

We need double differential, differential and total cross section experimental data to validate our models. There exist data from experiments performed for condensed matter physics, but should be used with some care:

- Measurements are sometimes qualitative.
- Sometimes not all data corrections were applied.

With this in mind, there is a wealth of data available from the different laboratories. A project should be set up to incorporate existing (and useful) thermal scattering data to EXFOR.

Recommendation II:

We should look back at the foundational efforts in thermal scattering evaluation (General Atomics group, IKE Stuttgart group):

- Combine condensed matter studies, with neutron sources and nuclear reactor applications. These are different disciplines now: the problem is interdisciplinary.
- There is not a single instrument to measure everything: total cross section measurements are simple and cost effective, but differential measurements give more information for validation.

Collaboration between communities should be encouraged and supported.

Recommendation III:

Modern evaluation trends set new requirements for experimental data [11]:

- Refinement of existing thermal scattering kernels, mainly driven by nuclear criticality calculations.
- New evaluations for advanced neutron sources and neutron filters.
- Covariance matrix generation for existing and new evaluations.

The different projects will eventually require and obtain new experimental data. EXFOR should promote and coordinate experimental activities, and incorporate the produced data.

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[1] Koppel, J.U., & Houston, D.H. *Reference Manual for ENDF Thermal Neutron Scattering Data (*Report GA-8774). Gulf General Atomic, Inc., San Diego, Calif. (1968*).*

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[7] Al-Qasir, I., Jisrawi, N., Gillette, V., & Qteish, A. *Thermal neutron scattering cross sections of beryllium and magnesium oxide*s. Ann. Nucl. Energy **87** (2016) 242-251.
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2.7 Y. Kiyanagi, Nagoya University: "Development of the Thermal Cross Section and its Necessity for Neutron Applications"

1. Contribution

Thermal neutron cross sections became more important than before since application areas are expanding such as neutron scattering, boron neutron capture therapy as well as reactor physics.

In Japan, water and heavy water thermal cross sections have been evaluated [1]. For the evaluation molecular dynamics was adopted to obtain more rigorous results. Evaluations were performed for 298K and 350K for water. Gaussian approximation for the width function gave rather good agreement compared with ENDF/B-VII. However, the assumption did not reproduce the jump diffusion nature of the water molecule diffusion. Therefore, new method, direct calculation of the Van Hove correlation function by MD with a new quantum correction GAAQC, was proposed. This method well reproduced the jump diffusion nature and improve the agreement with the experimental data. A result of the heavy water evaluation was also shown and it also gave good agreement with the experimental results.

As applications, simulations of the accelerator driven neutron sources and boron neutron capture therapy sources require the thermal neutron kernel, and recently in the neutron scattering field simulation of the scattering process requires the crystal scattering cross section. We recently developed a pulsed neutron imaging [2, 3] and it also requires the simulations to understand the experimental results and to consider the optimal experimental setup. A transmission experiment to indicate free water and bound water (hydrogen) in cement pastes by using the gradient of the total neutron cross section at low energy region was introduced as an example of the pulsed neutron imaging [4]. It was indicated by the simulation using the water and the ice cross section that multiple scattering affected the gradient of the total cross section and the effect made the gradient of water gentler. For the optimal setup for the crystal material such as iron, the distance from the sample to the detector was important and it was indicated by simulation that about 30 cm distance was required to reduce the scattering effect.

In Japan, there are several compact neutron sources that can be used for the total cross section and big facilities exist that can be used for inelastic scattering and diffraction measurements. The compact neutron sources are very useful for the total neutron cross section measurement due to its easy access. However, it is not so easy to get the beam time at the big facility. International support to promote

cross section measurements is preferable for promoting the thermal neutron cross section measurements.

2. Recommendations

a. Items that should be included in the EXFOR

Total neutron cross section

Experimental data of the total cross section are one of the fundamental information for evaluating the neutron cross section since it reflects all components affecting the cross section. The data should be compiled in EXFOR with comments on the experimental condition (purity, temperature, crystal material condition (powder (size), single crystal), and experimental resolution)

Double differential cross section and Structure factor S(Q)

S(Q) is necessary to validate models and methods adopted for evaluations. The data should also include the comments written in the total cross section. To refer the original paper is necessary.

However, the number of such data is enormous since the material scientists perform various kinds of inelastic scattering and diffraction experiments. Therefore, it will be required to select materials to be compiled. A guide line will be helpful for selecting materials. In the selection not only the reactor physics field, but also other fields such as the neutron therapy will be taken into account.

b. Data collection and comparison

New evaluations are performed and new data are being produced. However, there are data not yet compiled. Such information should be transferred to EXFOR. The number to be compiled have to be limited as mentioned before.

For this kind of activity a regular meeting by professional should be organized.

c. Neutron data revision

Many of the thermal kernels compiled in the data library were evaluated by using the old data around 1970s. At that time the neutron inelastic scattering machines and the diffraction machines were not as good as present ones. They might cover not enough energy regions and performed under poor resolution. In the thermal energy region, to evaluate the cross section we need many kinds of effects such as various dynamic modes, crystal structure and so on. So, the precise experimental data should be obtained by using modern machines.

Total cross section can be measured by using the compact pulsed neutron sources. Such facility can be used more easily than the big facilities. For the inelastic experiments and diffraction experiments we need bigger machine and we have to pass the review. However, it is usually not easy since the aim is rather conservative. International support, as from IAEA, is very helpful to promote such measurements.

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2.8 E. Farhi, Institut Laue-Langevin: "Combining Molecular Dynamics Simulation and Experiments to Improve Neutron Scattering Cross Section Data"

Outline of the presentation

A schematic view of different possibilities to obtain the neutron scattering cross section is presented. The main methodologies involve direct transmission measurements of the integrated total cross section, time-of-flight scattering experiments, molecular dynamics, and the simulated small displacement dynamical matrix estimate of the normal modes. Then, most methodologies can be

employed either to estimate the density of states as an input to e.g. NJOY/LEAPR models to evaluate the *S(q,w)* scattering law, or the direct determination of the *S(q,w)* dynamical structure factor. The integrated total cross section is further estimated from the integration of the double differential cross section.

The integrated total cross section measurement has not been discussed during this presentation, as it is the main focus of the talk by F. Cantargi.

The conventional methodology used so far is to measure the generalised density of states (gDOS, a.k.a. frequency or phonon spectrum) using a neutron time-of-flight spectrometer, and then use one of the many available models implemented in LEAPR to reconstruct (evaluate) the $S(\alpha,\beta)$ scattering law. This methodology has been validated by decades of usage and is widely accepted by the EXFOR end-user nuclear engineers' community. However, a limited number of such data sets currently exist in EXFOR, such as Be, BeO, H_2O, D_2O, ZrH_x, graphite, l-D_2, l-H_2, … as listed for instance in the INDC-NDS-0470 report (Mattes and Keinert, 2005) and the NJOY/LEAPR manual (McFarlane, 1994). As the models considered today mostly rely on the so-called Gaussian approximation, which depends solely on the density of states of the materials, no structural nor accurate phonon dispersion relations can be considered in this methodology. In this view, the $S(\alpha,\beta)$ models are mostly targeted to handle incoherent materials and recoil/ballistic free gas behaviours. However, the Sköld approximation can be used to infer the coherent scattering contribution from the incoherent part, with a surprisingly efficient and handy formalism. An inherent limitation of this methodology is that the generalised density of states is a crude approximation of the "true" vibrational density of states, is only justified for pure incoherent scatterers and moreover it cannot be properly evaluated in the limit $q \rightarrow 0$, due to the limited accessible dynamic range of any neutron instrument used for the measurement.

The development of modern high flux neutron time-of-flight spectrometers, with extensive detector coverage and variable incident neutron energy allows to directly measure the *S(q,w)* total scattering law. This type of measurement has proven to be reliable especially to obtain the low-*(q,w)* structural and dynamical information. Many materials have been measured but very few are referenced in EXFOR so far. One simple reason is that this methodology suffers from many limitations. This includes for instance noisy data sets, especially when the energy transfer gets significant and the signal reaches the instrument sensitivity level. Also, except when using polarised neutron beams, only the total scattering law can be measured, which overlaps coherent and incoherent contributions with few hopes to separate one from the other. The partial scattering law contributions from each atom composing e.g. molecules are then hardly available. Also, the data reduction steps required to produce the dynamical structure factor data implies a number of approximations which depend highly on the data processing methodology (normalisation, detector efficiency, empty cell, transmission and self-shielding corrections, multiple scattering subtraction, etc). One way to overcome this issue is to provide EXFOR with only the raw *I(q,t)* data sets, with as few as possible treatment steps and detailed experimental information used during the measurement. But the major limitation arises from the limited dynamic range which can be measured. This range is determined by the neutron energy and momentum selection rules, and is not rectangular in shape, hindering the capability to properly evaluate quantities such as the gDOS and the structure factor. In principle, the resulting data set is only valid for incident neutron energy lower than the one used during the experiment. In practice, the resulting experimental *S(q,w)* data sets can reach energy transfers up to a few 100 meV, to be compared with the requirements of 3-10 eV data needed for neutron moderation in nuclear applications.

A way to bypass these experimental limitations is to make use of molecular dynamics simulation results. Such a possibility is currently employed by the Bariloche team to better estimate the vibrational density of states of the molecular dynamics simulation trajectory from which the velocity auto-correlation function is computed, providing the "true" density of states. Then the conventional LEAPR models are used to generate the scattering law. The main advantage of this methodology is that it brings additional information from the molecular dynamics without reconsidering the full processing work-flow. However, as in the conventional methodology, the angular information (e.g. the momentum) is lost before inputting the density of states into LEAPR, so that the final momentum

distributions are only reconstructed after evaluation of selected models, and cannot obviously contain structural or dispersion relation information.

The molecular dynamics simulation results can also be used to fully compute the scattering law by a double Fourier transform. This methodology gives an alternative to the conventional method based on the density of states. It also provides the full structural (elastic) and dynamical (inelastic) information for both coherent and incoherent processes, and allows separating the contributions of each atom in molecules and compounds. Most materials can be simulated in a reasonable computational time, in order to obtain *S(q,w)* up to e.g. 0.5-1 eV energy, on a regular square *(q,w)* range which facilitates the evaluation of further integrated quantities. However, one limitation is that all molecular dynamics simulations are performed in the so-called classical approximation and provide a symmetrised scattering law. The detailed balance relation must then be applied to recover the true scattering law. Unfortunately, at large energy transfers (e.g. larger than 50 meV) the exponential thermal Boltzmann correction diverges. Additional corrections must then be applied to counter balance this divergence so that the simulated *S(q,w)* can be used to compare with experiments and compute the total integrated cross sections. As this methodology presents many advantages, it may be advisable to validate it against corresponding experimental data (e.g. static and dynamical structure factor). The simulated data set on a wide *(q,w)* range then can be converted to the (α,β) space for inclusion into EXFOR-type data bases.

Last, the small displacement molecular dynamics methodology has been mentioned as it provides a fast estimate of the dispersion relations in crystalline materials, which can be used as well for powders. The vibrational density of states can then be computed. This methodology, however only provide the coherent inelastic contribution so that other contributions must be evaluated by other methodologies.

In short, it is possible today to make use of raw experimental data, evaluated models and molecular dynamics simulations to compute the scattering law on complementary energy ranges. These methods are not exclusive and may be used consecutively to improve and cross-check the accuracy of the existing *S(a,b)* data sets.

Discussion

A general discussion regarding the type of experimental data to include in EXFOR, and the distinction between raw experimental data, e.g. *I(q)* (code DA) and *I(q,t)* (code DAE) which highly depend on the measurement details (instrument used and its main parameters), and the possibility to rather include more fundamental derived quantities such as *S(q)* and *S(q,w)*. The accurate specification of the instrument parameters and geometry is advisable in order to properly use any experimental data set.

Recommendations

1) The raw data, e.g. integrated cross section $\sigma(E_i)$, diffractogram $I(\theta)$, and angle time-of-flight spectrogram $I(\theta,t)$ should be preferred to processed data as they imply less corrections.
2) Accurate instrument parameters used during the measurements (or simulation) should be specified.
3) Processed data, e.g. gDOS, vDOS, $S(q)$, $S(q,\omega)$ could be stored in a new dedicated section of EXFOR.

3. Summary of discussions and recommendations

3.1 Summary of discussions

During the presentation of the talks it was pointed out that the EXFOR database currently does include only a few data sets related to neutron thermal scattering, and most of those data are old. For example, a search of double differential thermal neutron scattering data (n, *; DAE) only retrieves two datasets: one for Benzene and one for Beryllium. On the other hand, there is significant amount of

data already published that could be compiled and incorporated to EXFOR. These data has to be collected carefully because in many cases it was not produced with nuclear data in mind and it might not be suitable for validation.

Several common problems for the measurement and publication of new thermal scattering data were discussed between the participants. The users of large neutron scattering facilities reported it is often difficult to obtain beam time to perform experiments related to nuclear data because its significance is not recognized by the screening advisory the same problem was pointed out for the publication of new experimental data, which is sometimes rejected in journals, especially when measurements cover materials or quantities for which there exist old data. Contributors from small neutron sources emphasized the role that these facilities play in the production of new experimental data for thermal scattering library evaluation (particularly, total cross sections), their important share in the contributions that already exist in EXFOR, and the support that is needed to continue these activities.

Several neutron scattering techniques were presented by the participants, and their differences were discussed during the meeting, with a special focus on the dynamical range that could be accessible with each type of instrument. The effect of the different data correction and reduction methods (including normalization, background subtraction, multiple scattering corrections and inelasticity corrections) was discussed, along with the necessity of storing data at different levels of processing. Other experimental techniques, such as X-ray crystallography, IR and Raman spectrometry, that could produce experimental data useful for thermal scattering library evaluations were also analyzed.

The participants discussed the renewed interest placed upon the revision of existing thermal scattering libraries and the production of new evaluations driven by new applications, and also the activities already started within the Working Party on International Nuclear Data Evaluation Co-operation (WPEC) Subgroup 42: "Thermal Scattering Kernel S(α,β): Measurement, Evaluation and Application". These new activities place new requirements on experimental data, and eventually might produce it.

The different evaluation approaches used to produce new libraries and update existing ones were also discussed. This discussion included the characteristics of the different calculation methods, particularly the effect of molecular dynamics potentials (SPC, TIP4P) in the computed output, and the demands these methodologies place on experimental data.

Part of the meeting was dedicated to review the LEXFOR manual section on thermal scattering data, in particular to the collection of neutron scattering lengths. It was pointed out that there exist compilations of experimental data [1] and recommended data [2, 3, 4] that could be used as a source of definitions, experimental methods descriptions and data. The fields of the EXFOR database entries and its application to thermal scattering data storage and retrieval were also discussed, and a draft template to collect time of flight thermal scattering data was prepared.

Another point discussed was the physics of thermal scattering, and its differences from analysis of scattering in epithermal range. In thermal scattering the energy dependence of the nuclear neutron cross section is usually neglected (it is considered that only potential scattering occurs) and it is characterized as a constant scattering cross section; in the epithermal range the effect of absorption and scattering resonances is important, but the effects derived from condensed matter are usually considered only as free-gas Doppler broadening.

On the same line, the features that appear on differential and double differential scattering data and their relation to physical properties (elastic and quasielastic peaks, atom recoil) were discussed. It was also noted that in thermal scattering the focus is not only placed in the isotopes that compose the sample, but also in the compound, structure, phase, orientation, thermodynamics and other physical properties, and these aspects have to be considered in the compilation of experimental data.

References:

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3.2 Recommendations

It is well recognized by those using simulation codes for the design of nuclear reactors and other nuclear systems that the existing thermal neutron scattering evaluations are inadequate for many purposes. This comes primarily from the lack of relevant data for materials and/or conditions of interest, but also from the lack of fidelity of some existing data when applied to these "novel" situations. For instance, recent work in Japan found inaccuracies even in the resonance region for Cu, and many of the existing thermal scattering data sets in repositories which are based on data collected in the 1970s and 1980's. In contrast to the state of the art in those days, modern neutron scattering instruments are capable of providing data over a much wider range of energy and momentum transfer (typically simultaneously), and therefore hold promise for providing far more extensive raw data to support the data libraries. Unfortunately, the acquisition of the primary neutron scattering data that would be suitable for the construction of useful thermal nuclear data libraries is not generally given a high priority by the review committees that are typically responsible for allocating beam time at the major neutron scattering facilities throughout the world. For materials of particular priority, it will be important to make use of such instruments to provide the data needed to refine existing models in those cases where they have proven to be inadequate. However, it is unlikely that sufficient time will be available on such instruments over the next several years to produce a sufficient increase in the volume or quality of the thermal scattering data available for users of libraries such as EXFOR.

Nevertheless, it is important to recognize that neutron transport codes are being applied to an ever expanding range of applications (such as design of accelerator-driven neutron sources, developing treatment plans for neutron and proton radiotherapy, etc.). Therefore the need for adequate data sets on new materials to support simulations using these codes can be expected to expand over the next few decades. Both the range of materials for which suitable data libraries will be needed, and the methods for evaluating those data sets will have to expand to satisfy this increasing demand, and it is important that alternative routes to producing suitable data sets are found. We propose that this is an area where smaller neutron sources and modern materials simulation capabilities may be able to provide important contributions.

The specific recommendations to improve completeness and quality of data in EXFOR:

- Double differential cross section, differential cross section, and total cross section experimental data should be stored and details of the experiments and instruments shall be laid out clearly.

- Publish guidelines for what is needed for acceptable submissions to EXFOR (specify needed/suggested metadata including experimental details needed to understand the processing of the data). This should be provided as template for EXFOR data compilers.

- $S(q,\omega)$ or $S(\alpha, \beta)$ could be stored in a new dedicated section of EXFOR with details of the derivation being provided.

- Phonon spectrum, structural parameters, and other information derived from neutron double differential scattering experiments, X-ray crystallography and modelling should be stored in a separate repository accessible to the evaluators as derived data, with details of the derivation being provided.

- We recommend that the Nuclear Data Section consider reviewing the existing thermal scattering data evaluations, and coordinate/support activities to improve them and expand their applicability.

- The NRDC coordinator should encourage editors of suitable journals (Atomic Data and Nuclear Data Tables, Annals of Nuclear Energy, Nuclear Instruments and Methods A and B) to consider high-

quality work relevant to nuclear data applications even to the point of accepting new measurements on old materials.

- The Nuclear Data Section should consider the initiation of a project to compile existing experimental data for EXFOR, and suitable experimental and theoretical data for the input parameter repository regarding materials that are known to be important from the thermal scattering perspective.

- Modern evaluation trends set new requirements for experimental data:
  - Refinement of existing thermal scattering kernels, mainly driven by nuclear criticality calculations.
  - New evaluations for advanced neutron sources, neutron filters, BNCT, and other applications that may not be well served by evaluations based on nuclear criticality.
  - Covariance matrix generation for existing and new evaluations.

- A partial list of materials known to be of interest for thermal scattering library evaluation is provided in Table 1. This includes materials for which scattering kernels already exist, or are being considered for evaluation.

We recommend that EXFOR incorporate the experimental data produced by abovementioned demands.

We also recommend that the Nuclear Data Section consider the initiation of a project to coordinate measurements necessary to fulfil these needs. Particular emphasis should be placed upon the measurement of total cross sections in compact neutron sources, which are necessary for the evaluation effort and might not be covered by measurements performed for materials research.

Thermal-Neutron Scattering - LEXFOR Manual

Theory

The scattering of slow neutrons (energies less than the chemical binding energy, and not close to resonance region, typically less than a few eV), with matter depends on the atomic structure of the material (because the wavelength of slow neutrons is of the order of inter-atomic distances) and on the atomic dynamics in the scattering medium (because the energy of slow neutrons is of the same order as the energy of thermal motion of atoms in materials). Van Hove formulated the double differential cross sections considering the structure and dynamics as

$$d^2\sigma/d\Omega dE' = (1/2\pi\hbar)\,(k'/k)\,\Sigma_{ij}\, b_i b_j \int_{-\infty}^{+\infty} dt \langle \exp(-i\mathbf{q}\cdot\mathbf{r}_j(0))\exp(-i\mathbf{q}\cdot\mathbf{r}_i(t))\rangle_T \exp(-i\omega t)$$

where k and k' are the initial and final wave numbers of the neutron, b_i is the scattering length of the nucleus i which is at position $\mathbf{r}_i$ at time t,$\mathbf{q}=\mathbf{k'}-\mathbf{k}$ is the momentum transfer of neutron, and $\hbar\omega=E'-E$ is the energy transfer of neutron. $\langle ... \rangle_T$ denotes averaging over the canonical ensemble characterized by the temperature T. If we denotes the integral by $S_{ij}(\mathbf{q},\omega)$, and decompose the differential cross section to the $i\neq j$ and $i=j$ part:

$$d\sigma/d\Omega dE' = (1/2\pi\hbar)\,(k'/k)\,[\langle b\rangle^2 \Sigma_{i\neq j}\, S_{ij}(\mathbf{q},\omega) + \langle b^2\rangle \Sigma_{i=j}\, S_{ij}(\mathbf{q},\omega)]$$

$$= (1/2\pi\hbar)\,(k'/k)\,[\langle b\rangle^2 \Sigma_{i,j}\, S_{ij}(\mathbf{q},\omega) + (\langle b^2\rangle - \langle b\rangle^2) \Sigma_{i=j}\, S_{ij}(\mathbf{q},\omega)]$$

where $\langle b\rangle^2$ is $\langle b_i b_j\rangle$ with $i\neq j$ and $\langle b^2\rangle = \langle b_i b_j\rangle$ with $i=j$. The first term of the second equation involving all nuclear states (isotopes and spin states of the compound) describes **coherent scattering** while the second term involving a single nuclear state describes **incoherent scattering**.

Coding

- For all scattering processes where molecular and crystalline forces are involved the code THS is used in reaction SF3. For other processes (e.g., total), the modifier TMP is always added to indicate that the quantity is temperature dependent.
- When the compiler is aware that the quantity depends on the orientation of the sample (e.g., transmission for a single crystal), it must be indicated by SF8=MSC with free text.
- The sample temperature is given under the heading TEMP.
- The crystal structure of the sample is given under the keyword SAMPLE.

Coherent and incoherent scattering length

The quantities $b_{coh}=\langle b\rangle$ and $b_{inc}= (\langle b^2\rangle - \langle b\rangle^2)^{1/2}$ are known as the coherent and incoherent scattering length.

The scattering length for a **free atom** (mass number A) is a factor A/(A+1) smaller than that for a **bound atom**. Their distinction is important for light nuclides.

Some strong neutron absorbers (e.g., ^{113}Cd, ^{157}Gd) may have an imaginary part of the scattering length. The imaginary part of $\langle b\rangle$ is related with the absorption cross section by $\mathrm{Im}(\langle b\rangle)=k\sigma_{abs}(E)/4\pi$ (optical theorem) at $E\rightarrow 0$.

The scattering length b is related with the **scattering amplitude** f(E) by $b=-\lim_{E\rightarrow 0} f(E)$. (Sometimes scattering length is called as scattering amplitude.)

REACTION Coding: COH or INC in SF5 and AMP in SF6. IM in SF5 for imaginary part.

Examples:

(6-C-12(N,THS)6-C-12,BA/COH,AMP)
Bound atom coherent scattering length of ^{12}C
(23-V-51(N,THS)23-V-51,FA/INC,AMP)
Free atom incoherent scattering length of ^{51}V
(64-GD-157(N,THS)64-GD-157,COH/IM,AMP)
Imaginary part of coherent scattering length of ^{157}Gd

Contribution of potential scattering and resonance scattering

The bound atom scattering length is the sum of the contribution from potential scattering and all s-wave resonances:

$$[A/(A+1)]|b_{\pm}| = R' - [(A+1)/A]\,[\hbar/(8m)^{1/2}]\,\Sigma_{i\pm}\,[(\Gamma_{n,i}/E_{0,i}^{3/2}) - i\,(\Gamma_{n,i}\Gamma_{n}/2E_{0,i}^{5/2})],$$

where m is the neutron mass and $\hbar c/(8m)^{1/2}$~2277 fm $eV^{1/2}$. R' is the **potential scattering radius**, A is the mass number of the nuclei, $\Gamma_{n,i}$ and Γ_i are the neutron and total width of the i-the resonance at the resonance energy $E_{0,i.}$ $\Sigma_{\pm}$ means summation for all resonance having the same spin $J_{+}=I+1/2$ or $J_{+}=I-1/2$. Their weighted mean gives $<b>=g_{+}b_{+}+g_{-}b_{-}$ with $g_{\pm}=[2(I\pm1/2)+1]/[(2I+1)2]$, where I is the spin of the target nucleus

Note that only J=I+1/2 is possible for spin zero nuclei, and $b_{coh}=b_{+}$ and $b_{inc}=0$ for them. For example, thorium gives no incoherent scattering because it is enriched to thorium-232 and its ground state spin is zero.

Coherent and incoherent scattering cross section

The quantities $\sigma_{coh}=4\pi b_{coh}^{2}$ and $\sigma_{inc}=4\pi b_{inc}^{2}$ are known as the coherent and incoherent scattering cross section. Their values for bound and free atom are related by the factor A/(A+1). Their sum $4\pi(b_{coh}^{2}+b_{inc}^{2})$ gives the total scattering cross section of fixed nuclei.

Examples:

(6-C-12(N,THS)6-C-12,BA/COH,SIG)
Bound atom coherent cross section of ^{12}C
(23-V-51(N,THS)23-V-51,INC,SIG)
Incoherent cross section of ^{51}V

References

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Template for submission of time-of-flight spectra, from Refs [A-F]

A. EXPERIMENT DESCRIPTION

1. Main Reference		[A]
2. Facility/Instrument		[B]
3. Neutron production Neutron production beam Nominal average beam energy Nominal average peak current or reactor power Repetition rate (pulses per second) Pulse width Primary neutron production target Target nominal neutron production intensity		
4. Moderator Primary neutron source position in moderator Moderator material Moderator dimensions (internal) (thickness, height×width×depth,…) Density (moderator material) Temperature (K) Moderator-room decoupler (Cd, B, …)		
5. Other experimental details referred to the instrument Distance (m) (moderator –chopper) Distance (m) (chopper –sample) Distance (m) (sample –detector) (range with mean value if necessary) Angle of flight path to the moderator normal Neutron beam dimensions at sample position (mm × mm, diameter in mm, …) Range of incident energy possible Angular range for the instrument Overlap suppression (Filter material and thickness, chopper, …) Other fixed beam filters Additional information		[C]
6. Detector Type Material Surface Dimensions (mm × mm. diameter in mm, …) Thickness (mm)		
Distance from sample (m) (range with mean if necessary) Detector(s) position relative to neutron beam Detector(s) solid angle		

7. Sample Type (metal, powder, liquid, crystal) Temperature (K) Pressure (bar) Crystal or powder structure (e.g., single, grain and/or powder size) Chemical composition, phase Sample composition (at/b) Sample density (g/mm^3) Sample mass (g) Geometrical shape (cylinder, sphere, …) Orientation of the sample referring to the flight path Surface dimension (mm × mm, diameter in mm, …) Nominal thickness (mm) in beam Additional comment		[D]
8. Other experimental details referred to the dataset Incident energy or range (meV) Angular range for the measurement Containment description Other measurements performed (e.g., empty can or sample out for background, vanadium for detector calibration, filter for energy calibration) Additional comment		[E]
9. Data Reduction Procedure Dead time correction Back ground subtraction Flux determination (reference reaction, …) Normalization Detector efficiency Self-shielding Time-of-flight binning Angular grouping Multiple scattering Software Procedure before and after software implementation Additional comment		[F]
10. Response function Initial pulse Target / moderator assembly Detector		
11. Error analysis Source of uncertainties propagated to the total uncertainties		

B. DATA FORMAT

As applicable, each dataset will record the same: incident energy, scattered angle, temperature, and pressure.

Column	Content	Unit	Comment
1	Incident Energy	meV	Mandatory as applicable
2	Outgoing Energy	meV	Mandatory as applicable
3	Scattering Angle	degree	Mandatory as applicable
4	Experimental observable	b, b/sr, or b/(sr·eV)	Mandatory: Transmission, cross section or ratio
5	Total Uncertainty		Not mandatory, but strongly recommended
6	Uncorrelated uncertainty		Mandatory: Uncertainty due to counting statistics, for example
7	Additional information		Not mandatory
8	Additional information		Not mandatory
…	…		…
18	Additional information		Not mandatory

REFERENCES

[A] The main reference for the work (website, journal, saved documents, or private communications) is mandatory.

[B] The reference for the facility and/or instrument (website, journals, and/or saved documents) is mandatory.

[C] The reference for other experimental details (website, journals, and/or saved documents) can substitute the entry in the same section.

[D] The reference for details of sample (website, journals, and/or saved documents) can substitute the entry in the same section.

[E] If needed, the reference for details of containment (website, journals, and/or saved documents) can be provided.

[F] The reference for details of reduction (website, journals, and/or saved documents) is mandatory and is very important.

Materials of interest for thermal scattering data compilation

Thermal moderators	Cold moderators	Structural materials	Neutron filters	Nuclear Fuel	Other applications
H_2O	Liquid H_2	Al	Silicon	UO_2	Hydrogen in water and biological materials for dosimetry.
D_2O	Liquid D2	Fe	Sapphire (Al_2O_3)		
CH_2	Solid D_2	Zr	Polycrystalline alumina		
C_6H_6	Liquid CH_4		Bismuth		
Plexiglass (polymethyl metacrylite)	Solid CH_4 (Phase I and II)		Silica		
Ethanol	CD_4				
Dowtherm	Clathrate				
Zr hydride	Solid Mesitylene				
Y hydride	Mesitylene/ Toluene				
Ce hydride	Liquid Ethane				
Mg hydride	Triphenylmethane				
Ti hydride	Liquid He-4 (for UCN)				
Lexan (polycarbonate)	Deuterated aromatics				
Dodecane	Ice				
Tributylphosphate	Heavy water ice				
Mesitylene	Ar				
Graphite					
Be					
BeO					
HF					
Teflon (C_2F_4)					

AGENDA

Consultants' Meeting on

"**Experimental Nuclear Reaction Data (EXFOR) Compilation of Thermal Neutron Scattering Data**"

2-4 November 2015

VIC, Room M0E68, IAEA Headquarters, Vienna, Austria

Monday, 2 November 2015

09:30 -10:45	**Opening Session** Administrative Announcements **(Alexander Oechs)** Self-introduction of **Participants** Welcome address **(Arjan Koning)** Welcome address **(Stanislav Simakov)** Selection of **Chairperson and Rapporteur** Approval of Agenda Objectives of the Meeting (**Valentina Semkova)**
Presentations *(presentations' time include questions and discussion)*	
11:00-11:45	**Naohiko Otsuka, IAEA-NDS** "Basic questions on compilation of experimental thermal neutron scattering data"
11:45 -12:30	**D.V. Baxter, Indiana University** "Compact Accelerator-driven Neutron Sources as tools for nuclear data"
12:30 -14:00	Lunch break
14:00 -14:45	**Li (Emily) Liu, Rensselaer Polytechnic Institute** "Thermal Neutron Scattering Measurements at Spallation Neutron Source and Analysis"
14:45 -15:30	**F. Cantargi, Centro Atomico Bariloche** "Total neutron cross section measurement for thermal scattering library evaluation"
16:00 -16:45	**J.I. Marquez Damian, Centro Atomico Bariloche** "Experimental data needs for thermal scattering library evaluation"
16:45 -17:30	**Y. Kiyanagi, Nagoya University** "Development of the thermal cross section and its necessity for neutron applications"

Tuesday, 3 November 2015

09:00 -09:45	**E. Farhi, Institut Laue-Langevin** "Combining molecular dynamics simulation and experiments to improve the S(a,b) low energy accuracy for improved neutron scattering cross sections"
09:45 -10:30	**Naohiko Otsuka, IAEA-NDS** "Revised draft of LEXFOR "thermal neutron scattering""
10:30 – 12:30	Discussions and drafting of Conclusions & Recommendations
12:30 -14:00	Lunch break
14:00 – 17:30	Discussions and drafting of Conclusions & Recommendations
19:00 -	**Social event:**

Wednesday, 4 November 2015

09:00 – 12:30	Discussions and Drafting of Conclusions & Recommendations
12:30 -14:00	Lunch break
14:00 -	**Final Remarks and End of the Meeting**.

IAEA
International Atomic Energy Agency
Atoms for Peace

LIST OF PARTICIPANTS

Consultants' Meeting on

"**Experimental Nuclear Reaction Data (EXFOR) Compilation of Thermal Neutron Scattering Data**"

2-4 November 2015

VIC, Room M0E68, IAEA Headquarters, Vienna, Austria

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