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SG42 Summary
&
Proposal for Subgroup on

Advances in Thermal Scattering Law Analysis

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SG42 Final Report

Thermal Scattering Law S(α,β)
Measurement, Evaluation and Application

International Evaluation co-operation

Volume 42

Executive summary

Simulation of nuclear systems requires a variety of data depending on the typical energies of the active particles. For many well-known systems, such as Light Water, Heavy Water or Graphite-Moderated Reactors, cold neutron source facilities (e.g. spallation neutron sources), and others, neutrons are slowed down to low energies where the chemical structure of materials plays a central role in the neutron physics. The simulation of thermalised systems is highly sensitive to neutron scattering and the quality of this data is of great importance and thermal scattering is a specialised discipline within the nuclear data community. Over the past two decades, great advances have been made in to use of atomistic simulation techniques including density functional theory (DFT) and molecular dynamics (MD) that, alongside the increase in computational power have provided a wealth of theoretical information for thermal scattering evaluation. Combined with new experimental data obtained in the past decade, this has resulted in an active area of research and a WPEC subgroup was launched to co-ordinate international activities.

This project stimulated numerous activities, resulting in, directly or indirectly, a suite of new evaluated thermal scattering law data evaluations that have been adopted in the most recent nuclear data libraries of the US (ENDF/B-VIII.0, February 2018) and the NEA Data Bank (JEFF-3.3, November 2017). This includes new evaluations for novel materials such as uranium nitride (UN), silicon carbide (SiC), silicon oxide (SiO_2) and aluminium oxide (Al_2O_3), as well as re-evaluation of critical materials including water (H_2O) and heavy water (D_2O) and enhanced evaluations including graphite at multiple levels of porosity and phase I_h ice. New evaluation techniques have provided additional data that were previously unavailable, including correlated uncertainties. New frontiers have been established through this subgroup, including the development and utilisation of these new data, the application of novel techniques to new system and use of the most recent experimental data, which will be addressed in future WPEC activities.

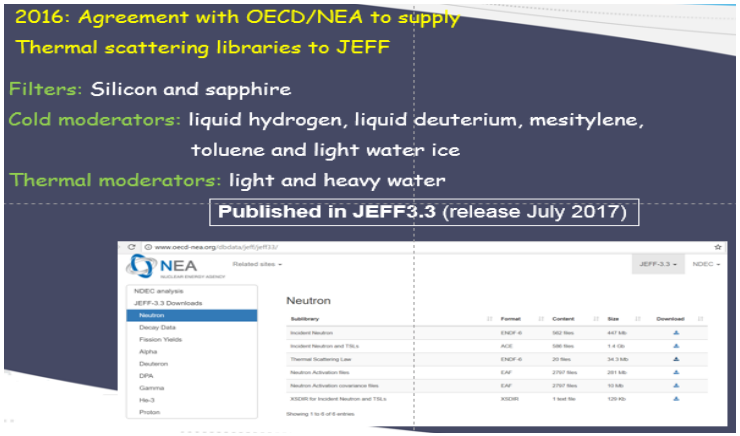
Members of WPEC/SG42 subgroup in attendance at the last meeting in May, 2018 at OECD/NEA headquarters in Paris, France. From left to right Atsushi Kimura (Japan Atomic Energy Agency, Japan), Michael Zerkel (Naval Nuclear Laboratory, USA), Jesse Holmes (Naval Nuclear Laboratory, USA), David Heinrichs (Lawrence Livermore National Laboratory, USA), Ayman Hawari (SG42 Monitor, North Carolina State University, USA), Gilles Noguere (SG42 Co-ordinator, CEA/DEN Cadarache, France), Li (Emily) Liu (Rensselaer Polytechnic Institute, USA), Danila Roubtsov (Canadian Nuclear Laboratory, Canada), Ivo Kodeli (Josef Stefan Institute, Slovenia), Luiz Leal (IRSN Fontenay-aux-Roses, France), Vaibhav Jaiswal (seated, IRSN Fontenay-aux-Roses, France), Florencia Cantargi (seated, Centro Atomico Bariloche, Argentina). Other contributing members who are not in the photo include but are not limited to: Yaron Danon (Rensselaer Polytechnic Institute, USA) and Jose Ignacio Márquez Damian (Centro Atomico Bariloche, Argentina).

SG42 TSL Evaluations

⇒ **Largest historical contribution of TSL evaluations**
⇒ **More than 50% are first-of-a-kind evaluations**

Table 2. New and updated TSL libraries in the ENDF/B-VIII.0 and JEFF-3.3 releases contributed by North Carolina State University (NCSU), Centro Atómico Bariloche (CAB), Canadian Nuclear Laboratories (CNL) and Bettis Atomic Power Laboratory (BAPL).

Material	Evaluation Basis	Institution	Library
Beryllium metal	DFT/LD	NCSU	ENDF/B-VIII.0
Beryllium oxide (beryllium)	DFT/LD	NCSU	ENDF/B-VIII.0
Beryllium oxide (oxygen)	DFT/LD	NCSU	ENDF/B-VIII.0
Polymethyl Methacrylate (Lucite)	MD	NCSU	ENDF/B-VIII.0
Polyethylene (hydrogen)	MD	NCSU	ENDF/B-VIII.0
Crystalline graphite	MD	NCSU	ENDF/B-VIII.0
Reactor graphite (10% porosity)	MD	NCSU	ENDF/B-VIII.0
Reactor graphite (30% porosity)	MD	NCSU	ENDF/B-VIII.0
Silicon carbide (silicon)	DFT/LD	NCSU	ENDF/B-VIII.0
Silicon carbide (carbon)	DFT/LD	NCSU	ENDF/B-VIII.0
Silicon dioxide (alpha phase)	DFT/LD	NCSU	ENDF/B-VIII.0
Silicon dioxide (beta phase)	DFT/LD	NCSU	ENDF/B-VIII.0
Uranium dioxide (oxygen)	DFT/LD	NCSU	ENDF/B-VIII.0
Uranium dioxide (uranium)	DFT/LD	NCSU	ENDF/B-VIII.0
Uranium nitride (nitrogen)	DFT/LD	NCSU	ENDF/B-VIII.0
Uranium nitride (uranium)	DFT/LD	NCSU	ENDF/B-VIII.0
Light water ice Ih (hydrogen)	DFT/LD	BAPL	ENDF/B-VIII.0
Light water ice Ih (oxygen)	DFT/LD	BAPL	ENDF/B-VIII.0
Yttrium hydride (hydrogen)	DFT/LD	BAPL	ENDF/B-VIII.0
Yttrium hydride (yttrium)	DFT/LD	BAPL	ENDF/B-VIII.0
Light water (hydrogen)	Exp. Data / MD	CAB, CNL	ENDF/B-VIII.0
Heavy water (deuterium)	Exp. Data / MD	CAB, CNL	ENDF/B-VIII.0, JEFF-3.3
Heavy water (oxygen)	Exp. Data / MD	CAB, CNL	ENDF/B-VIII.0, JEFF-3.3
Sapphire (aluminium)	Exp. Data / Debye model	CAB	JEFF-3.3
Sapphire (oxygen)	Exp. Data / Debye model	CAB	JEFF-3.3
Ortho-deuterium	Exp. Data	CAB	JEFF-3.3
Para-deuterium	Exp. Data	CAB	JEFF-3.3
Light water ice Ih (hydrogen)	Exp. Data	CAB	JEFF-3.3
Mesitylene Ph. II (hydrogen)	Exp. Data	CAB	JEFF-3.3
Ortho-hydrogen	Exp. Data	CAB	JEFF-3.3
Para-hydrogen	Exp. Data	CAB	JEFF-3.3
Toluene Ph. II (hydrogen)	Exp. Data	CAB	JEFF-3.3
Silicon	Exp. Data / Debye model	CAB	JEFF-3.3



SG42 recommendations

1) **Support the development of open source tools for thermal scattering data evaluation and processing with focus on providing nuclear data on demand at operational conditions.**
2) **Strengthen the collaboration with the neutron science and advanced neutron source communities (SNS, ESS, ILL, ISIS) in each country to establish joint experimental programs.**
3) **Support the data collection effort by EXFOR both in thermal scattering nuclear reaction data and supplementary material.**
4) **Identify and select sets of benchmark experiments that most appropriate for supporting the TSL evaluation process.**
5) **Converge on a modern format for TSL data in consultation with the GNDS effort.**
6) **Study the accuracy requirements for TSL evaluations, data processing and utilization.**

Consequently, during the last session of SG42, the participants unanimously recommended the start of a follow-up subgroup to continue the coordination of the international effort in TSL development and evaluation. This recommendation was also supported by entire WPEC body in the meeting held on May 20, 2018.

TSL SG Proposal

Advances in Thermal Scattering Law Analysis

- ⇒ **Continued growth in the area of thermal neutron scattering data motivates the formation of a new subgroup within the WPEC nuclear data collaboration**
  - ⇒ **The subgroup would be essential to continue international coordination on development and review of advanced TSL methods**
  - ⇒ **Act as the focal point with other WPEC subgroups (SG44, SG45, GNDS, etc.) in relation to data validation, covariance generation, and data formats, …**
  - ⇒ **Follow-up on the recommendations of SG42**
  - ⇒ **Motivate the TSL evaluation effort in support of various nuclear science and engineering applications**
    - ⇒ **Advanced reactors (e.g., various molten salts)**
    - ⇒ **Criticality safety (e.g., various U and Pu based fuels)**
    - ⇒ **Neutron science (e.g., cryogenic moderators)**

TSL SG Proposal

Advances in Thermal Scattering Law Analysis

Time-Schedule and Deliverables

- ⇒ **2020-2021: Review and documentation of advances in TSL evaluation methods and tools. Consideration will be given to emerging modern nuclear science and technology analysis modalities.**
- ⇒ **2021-2022: Review and documentation of TSL data validation, uncertainties and formats.**
- ⇒ **2022-2023: Summary and formulation of the SG findings, conclusions and recommendations.**

During the 3-year period, discussion of new and upcoming TSL evaluations, that are being considered for release into the databases (ENDF, JEFF, etc.), will continue. In addition, coordination with other WPEC subgroups will be ongoing.