WPEC Subgroup 48

Advances in Thermal Scattering Law Analysis

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32nd Meeting of the
NEA Working Party on International Nuclear Data Evaluation Co-operation
May 11 – 15, 2019 • WebEx Meeting

WPEC Subgroup 48
Agenda

Duration	PDT (CA, USA)	CEST (Paris)	JST (Tokyo)	Topic	
00:20	04:30	**13:30**	20:30	Welcome	A. Hawari, G. Noguère
00:20	04:50	**13:50**	20:50	Status of the TSL activities in the framework of the Nausicaa collaboration	G. Noguère
00:20	05:10	**14:10**	21:10	TSL measurement capabilities at ISIS	S. Lilley
00:20	05:30	**14:30**	21:30	Effect of thermal resonant treatment on keV scattering cross sections	R. Dagan
00:20	05:50	**14:50**	21:50	**Short break**	
00:20	06:10	**15:10**	22:10	The impact of uncertainty in thermal scattering on nuclear reactor parameters	L. Snoj
00:20	06:30	**15:30**	22:30	TSL Research at NSCU	A. Hawari
00:20	06:50	**15:50**	22:50	Validation of Thermal Scattering Laws for Light Water at Elevated Temperatures with Diffusion Experiments	J. Holmes
00:30	07:10	**16:10**	23:10	Discussion	
	07:40	**16:40**	23:40	Close	

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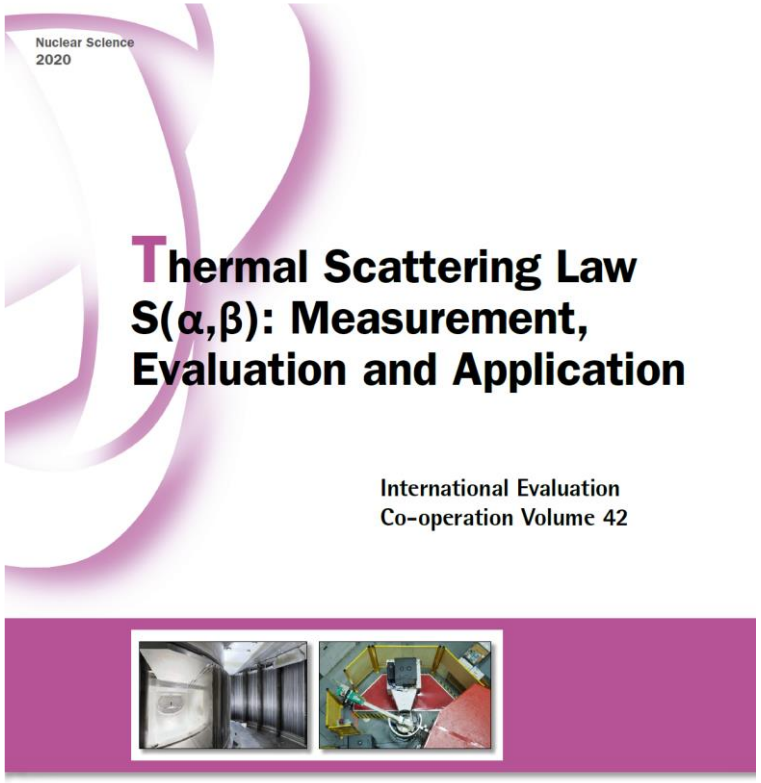

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SG42 TSL Evaluations

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

Table 4.1. **New and updated TSL libraries in the ENDF/B-VIII.0 and JEFF-3.3 releases contributed by NCSU, CAB, CNL and 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 I_h (hydrogen)	DFT/LD	BAPL	ENDF/B-VIII.0
Light water ice I_h (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 I_h (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

Notes: NCSU – North Carolina State University; CAB – Centro Atómico Bariloche; CNL – Canadian Nuclear Laboratories; BAPL – Bettis Atomic Power Laboratory; DFT – density functional theory; LD – Lattice dynamics; MD – Molecular dynamics; ENDF – Evaluated Nuclear Data File; JEFF – Joint Evaluated Fission and Fusion File.

JEFF-3.3 Thermal Scattering Law (TSL) sublibrary

The **JEFF-3.3 thermal neutron scattering sublibrary** contains 20 evaluations for 16 materials. Notably, the evaluation for heavy water is updated and now has components for deuterium and oxygen bound in heavy water. Nine new materials (sapphire- Al_2O_3, silicon, mesitylene, toluene, ortho- and para- hydrogen, ortho- and para-deuterium, and light water ice) have been included in this release. The remaining evaluations are carried forward from JEFF-3.2.

The origin of the new or updated JEFF-3.3 TSL evaluations is summarized below.

Thermal scattering libraries included in JEFF 3.3.

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Continued growth in the area of thermal neutron scattering data motivates the formation of a new subgroup within the WPEC nuclear data collaboration

- ⇒ **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)**
- ⇒ **Review the development of advanced TSL evaluation methods and tools with consideration of modern simulation approaches**
- ⇒ **Address issues related to data validation, covariance generation, and data formats, …**
- ⇒ **Act as the focal point with other WPEC subgroups (SG44, SG45, GNDS, etc.)**

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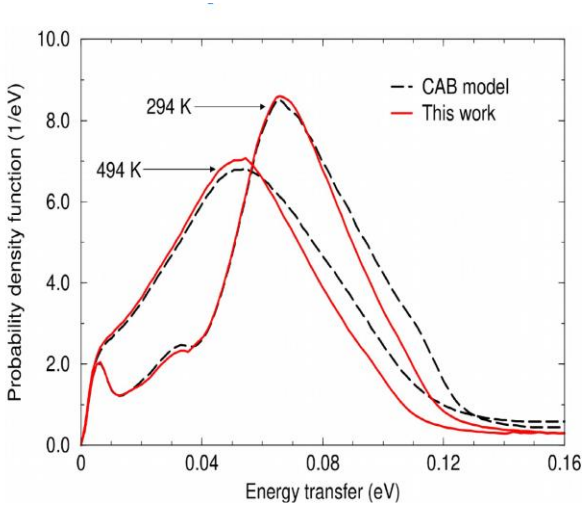

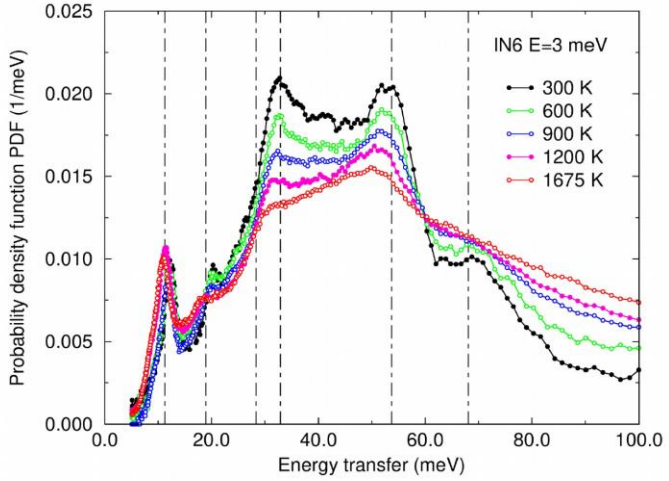

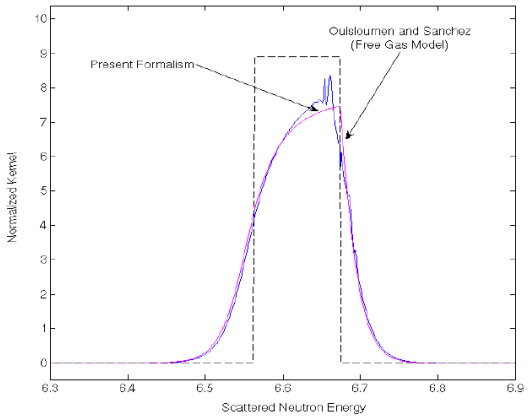

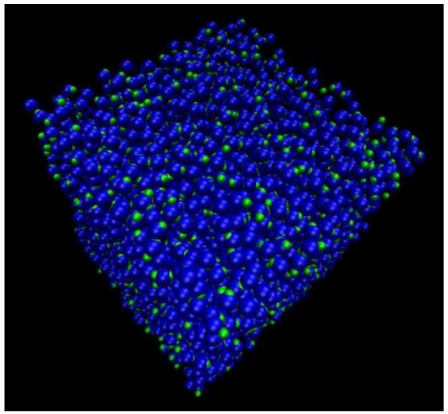

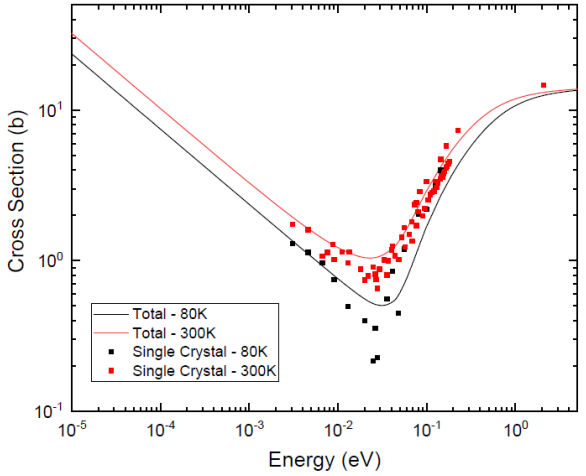

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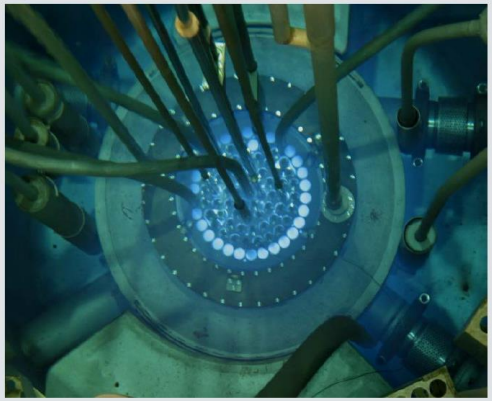

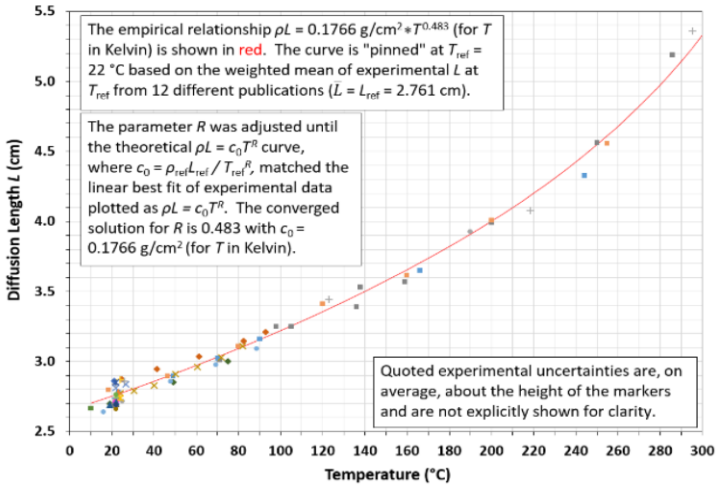

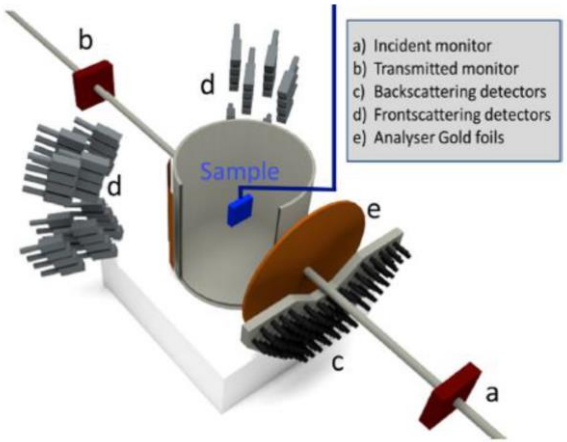

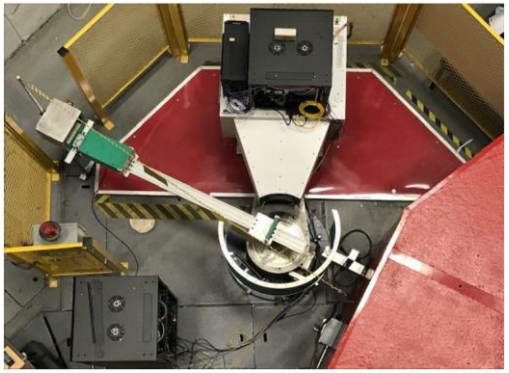

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Time-Schedule and Deliverables

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. Coordination with other WPEC subgroups will be ongoing.

In addition, the following deliverables will be pursued

- ⇒ **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.**

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Thank You