

**30th Meeting of the
NEA Working Party on International Nuclear Data Evaluation Co-operation
May 17 – 18, 2018 • Paris, France**

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Meeting Summary

SG42

Thermal Scattering Kernel $S(\alpha, \beta)$: Measurement, Evaluation and Application

Ayman Hawari, Gilles Noguere

SG42 Final Report

Thermal Scattering Kernel $S(\alpha, \beta)$ Measurement, Evaluation and Application

1) Context

2) Theory: evaluation methods and tools

- 2.1) Thermal Scattering Law definition
- 2.2) Main physics approximations used in LEAPR
- 2.3) Improved TSL libraries using atomistic simulations
- 2.4) A step forward for future TSL evaluations

3) Experimental validation

- 3.1) Material properties
- 3.2) Microscopic data
- 3.3) Semi-Integral data
- 3.4) Integral data
- 3.5) Facilities for TSL experiments
- 3.6) Capability gaps

4) Evaluation: progress on various materials and recent contributions to databases

- Reactor applications
- Criticality applications
- Neutron beam applications
- Cold neutron sources

5) Data format issues

- 5.1) TSL library format
- 5.2) TSL uncertainties

6) Summary and recommendations

APPENDIX if needed, such as LEAPR inputs and MCNP inputs of interest for this work



Development of evaluation methods and tools

⇒ The major development over the past 20 years is the implementation of atomistic simulation methods to support TSL evaluation

TABLE XLVII: Summary of the origins of and recent changes to the thermal neutron scattering (**thermal_scatt**) sublibrary. Evaluations modified for ENDF/B-VIII.0 are given in bold. Note all files were modified to correct the MAT numbering of the sublibrary.

File name	Main source	Last mod.	Lab.	Year	Note
tsl-ortho-D.endf	ENDF/B-VII.0	2016	LANL	1993	
tsl-para-D.endf	ENDF/B-VII.0	2016	LANL	1993	
tsl-ortho-H.endf	ENDF/B-VII.0	2016	LANL	1993	
tsl-para-H.endf	ENDF/B-VII.0	2016	LANL	1993	
tsl-013_Al027.endf	ENDF/B-VII.0	2016	LANL	2005	
tsl-026_Fe056.endf	ENDF/B-VII.0	2016	LANL	2005	
tsl-Be-metal.endf	ENDF/B-VIII.0	2016	NCSU	2016	DFT/AILD
tsl-BeInBeO.endf	ENDF/B-VIII.0	2016	NCSU	2016	DFT/AILD
tsl-OinBeO.endf	ENDF/B-VIII.0	2016	NCSU	2016	DFT/AILD
tsl-HinH2O.endf	ENDF/B-VIII.0	2016	CAB (Argentina)	2016	MD
tsl-HinIceIh.endf	ENDF/B-VIII.0	2016	BAPL	2016	DFT/AILD
tsl-OinIceIh.endf	ENDF/B-VIII.0	2016	BAPL	2016	DFT/AILD
tsl-DinD2O.endf	ENDF/B-VIII.0	2016	CAB (Argentina)	2016	MD
tsl-OinD2O.endf	ENDF/B-VIII.0	2016	CAB (Argentina)	2016	MD
tsl-benzene.endf	ENDF-269	2017	GA	1969	Corrected spelling; No LEAPR inputs available
tsl-HinC5O2H8.endf	ENDF/B-VIII.0	2016	NCSU	2015	MD
tsl-HinCH2.endf	ENDF/B-VIII.0	2016	NCSU	2015	MD
tsl-L-CH4.endf	ENDF/B-VII.0	2016	LANL	1993	
tsl-s-CH4.endf	ENDF/B-VII.0	2016	LANL	1993	
tsl-graphite.endf	ENDF/B-VIII.0	2016	NCSU	2016	DFT/AILD
tsl-reactor-graphite.endf	ENDF/B-VIII.0	2016	NCSU	2016	DFT/AILD
tsl-CinSiC.endf	ENDF/B-VIII.0	2016	NCSU	2014	DFT/AILD
tsl-SinSiC.endf	ENDF/B-VIII.0	2016	NCSU	2014	DFT/AILD
tsl-SiO2-alpha.endf	ENDF/B-VIII.0	2016	NCSU	2011	DFT/AILD
tsl-SiO2-beta.endf	ENDF/B-VIII.0	2016	NCSU	2011	DFT/AILD

TABLE XLVII: Summary of the origins of and recent changes to the thermal neutron scattering (**thermal_scatt**) sublibrary. Evaluations modified for ENDF/B-VIII.0 are given in bold. Note all files were modified to correct the MAT numbering of the sublibrary.

File name	Main source	Last mod.	Lab.	Year	Note
tsl-HinYH2.endf	ENDF/B-VIII.0	2016	BAPL	2016	DFT/AILD
tsl-YinYH2.endf	ENDF/B-VIII.0	2016	BAPL	2016	DFT/AILD
tsl-HinZrH.endf	ENDF/B-VII.0	2016	LANL	1993	
tsl-ZrinZrH.endf	ENDF/B-VII.0	2016	LANL	1993	
tsl-OinUO2.endf	ENDF/B-VIII.0	2016	NCSU	2016	DFT/AILD
tsl-UinUO2.endf	ENDF/B-VIII.0	2016	NCSU	2016	DFT/AILD
tsl-NinUN.endf	ENDF/B-VIII.0	2017	NCSU	2017	DFT/AILD
tsl-UinUN.endf	ENDF/B-VIII.0	2017	NCSU	2017	DFT/AILD

At the beginning of 2018, light and heavy water cross section libraries were published in ENDF/B-VII.0



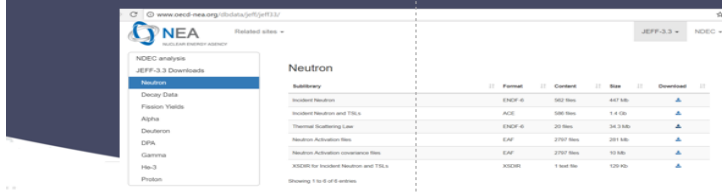
2016: Agreement with OECD/NEA to supply Thermal scattering libraries to JEFF

Filters: Silicon and sapphire

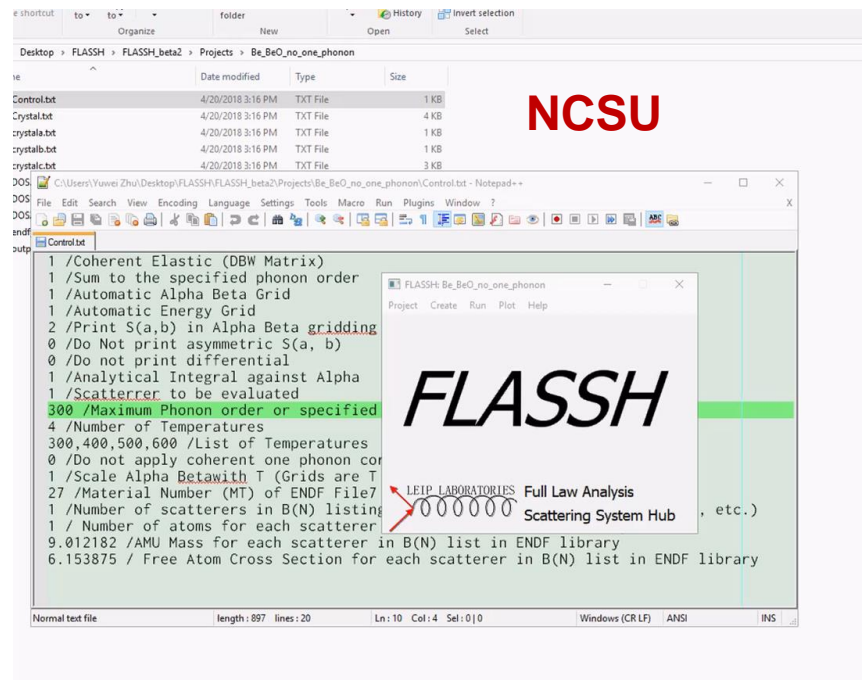
Cold moderators: liquid hydrogen, liquid deuterium, mesitylene, toluene and light water ice

Thermal moderators: light and heavy water

Published in JEFF3.3 (release July 2017)

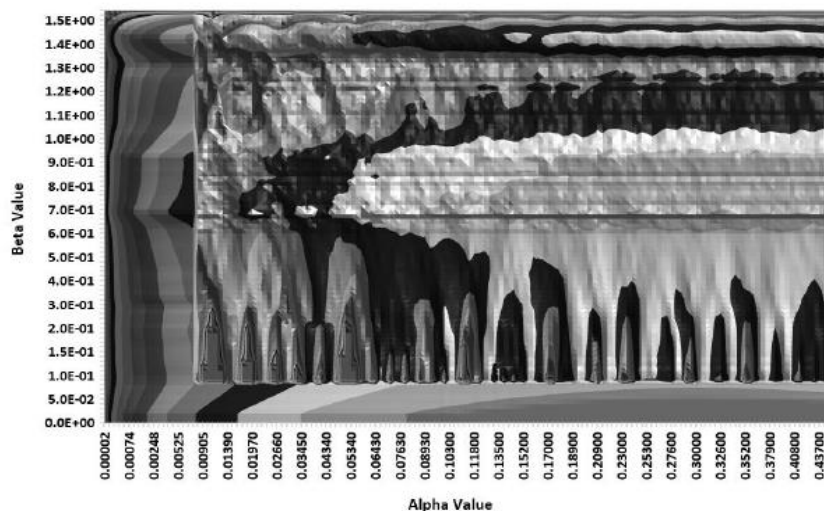


Development of evaluation methods and tools

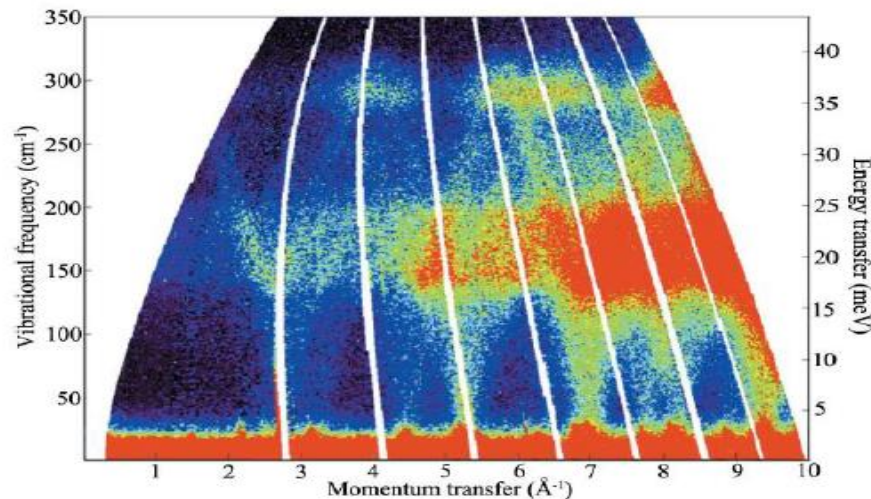
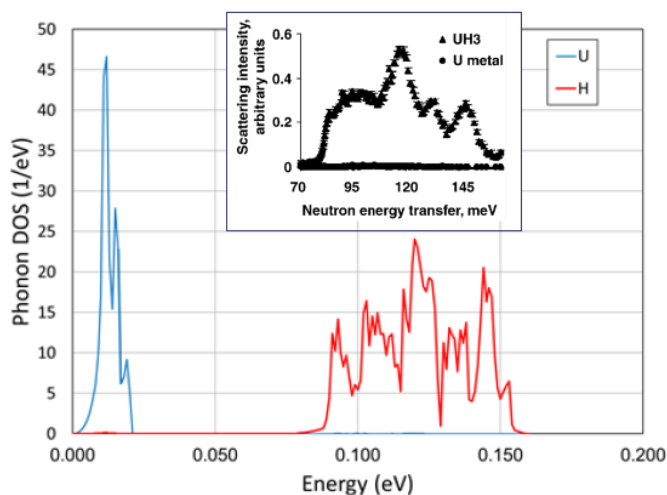


NCSU

One-Phonon $S(\alpha, \beta)$ for Aluminum with Coherent Interference
(calculated with MedeA and FLASSH)



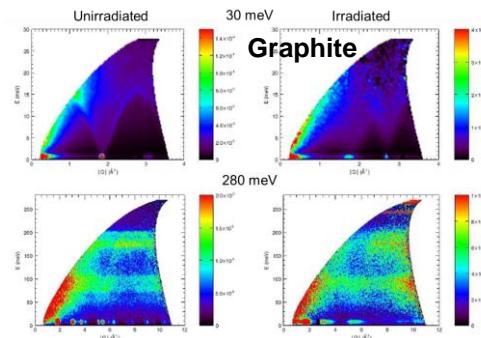
Calculated Phonon DOS for UH_3



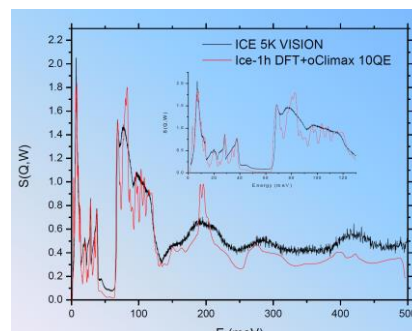
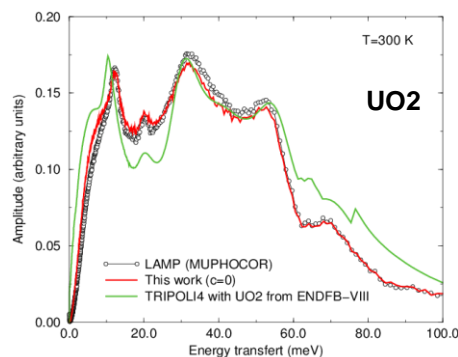
Experimental data from: Roach et al., J. Appl. Cryst. (2003)

Theory-Measurements Connections

- ⇒ Experimental validation of the double-differential neutron cross sections using TOF chopper spectrometers (inelastic measurements)
- ⇒ Experimental validation of the neutron total cross section using transmission technique
- ⇒ Experimental validation using pulsed slowing down and die away experiments
- ⇒ Experimental validation using integral benchmarks



Lawrence Livermore National Laboratory (LLNL)
Proof-of-Principle PNDA Experiment



Data covariance information and formats

Agenda

WPEC Subgroup 42

Thermal Scattering Kernel $S(\alpha, \beta)$:
Measurement, Evaluation and Application
and

WPEC Subgroup 44

Investigation of Covariance Data
in General Purpose Nuclear Data Libraries
and

WPEC Expert Group GNDS

Expert Group on the Recommended Definition of a
General Nuclear Database Structure (GNDS)

OECD Headquarters
Conference Center
2 Rue André Pascal,
Paris 75016

Room Chateau E

Starting at 2:00 pm – Ending at 18:00 pm

GNDS-1.9 & future TSL formats



Incoherent approximation of
 $S(\alpha, \beta)$ supported as in ENDF-6

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      <freeAtomCrossSection value="9.283302" unit="b"/>
      <e_critical value="197.6285" unit="eV"/>
      <e_max value="5.000001" unit="eV"/>
      <T_effective>=
    </scatteringAtom>
  </scatteringAtoms>
  <S_alpha_beta>...</S_alpha_beta>
</incoherentInelastic>
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Proposal: A **new subgroup on Advanced 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 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, ...**