Update on Naval Nuclear Laboratory TSL Evaluations

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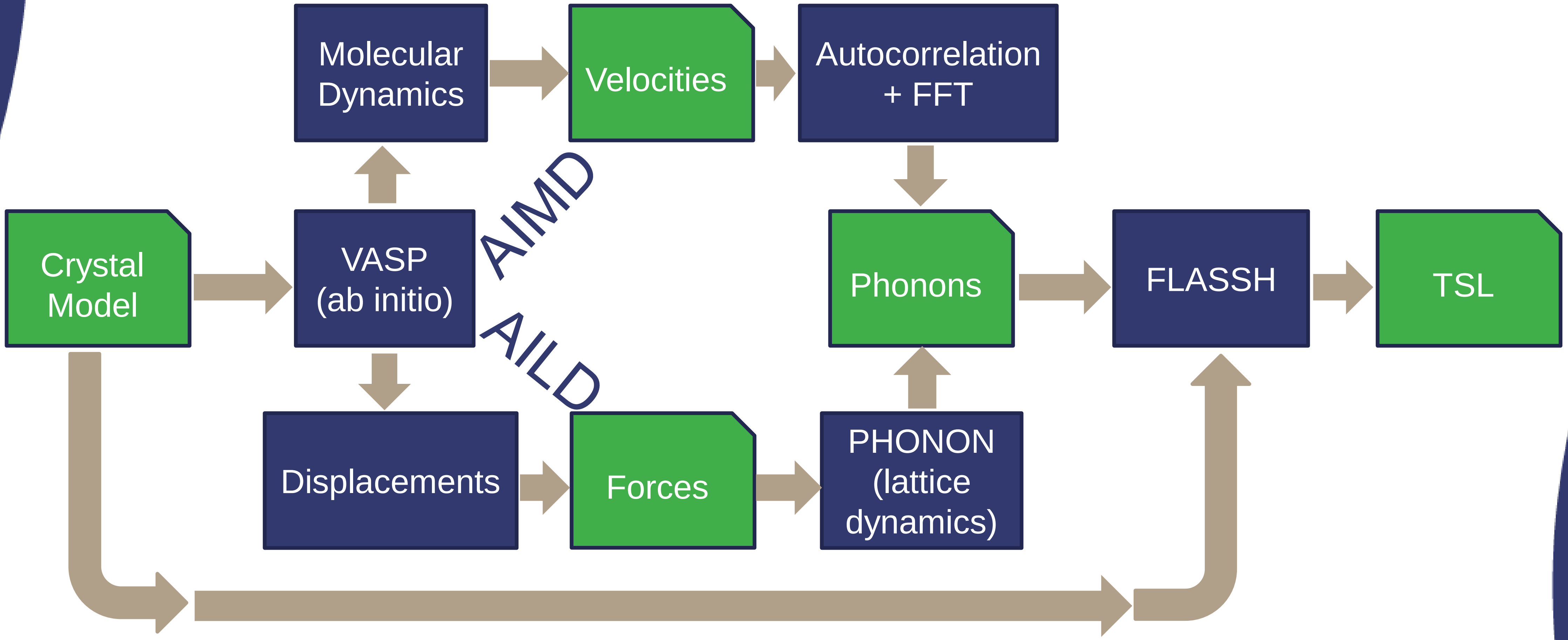
NAVAL NUCLEAR LABORATORY

Overview

- New TSL evaluations and re-evaluations for submission to ENDF/B-VIII.1
  - Solid moderator systems
  - Several quantum oscillators
    - Quantized oscillations in TSL as a function β
- Materials of interest for advanced reactors and criticality safety applications
- Exclusive use of FLASSH
  - *Ab initio* methods for phonons
  - Generalized coherent elastic
  - Mixed elastic scattering
  - Disordered alloy theory
  - Incoherent approximation
- New processing methods

TSL Evaluation Methods



New Methods in TSL Evaluations

- *Ab initio* molecular dynamics
  - Advanced method to generate phonon spectra[1,2]
  - Uses predictive *ab initio* force field
  - Captures anharmonicity neglected in ENDF/B-VIII.0 with *ab initio* lattice dynamics

- Mixed elastic scattering format
  - Combined use of coherent and incoherent elastic scattering on MT=2 [3]

- Disordered alloy theory
  - Improved treatment isotopic composition effect on coherent elastic scattering[4]
  - Currently being applied to Zr

1. J.L. Wormald and A.I. Hawari, *EPJ Web of Conf.* **146**, 13002 (2017) https://doi.org/10.1051/epjconf/201714613002
2. J.L. Wormald and A.I. Hawari, *Prog. Nucl. Energy* **101**, 461 (2017) https://doi.org/10.1016/j.pnucene.2017.02.011
3. M.L. Zerkle, CSEWG 2020 (https://indico.bnl.gov/event/7233/contributions/43822/attachments/31592/49906/Mixed_Elastic_Scattering_Format.pdf)
4. J.L. Wormald, J.C. Holmes, and M.L. Zerkle, *NSE* (2022) (*accepted*) https://https://doi.org/10.1080/00295639.2022.2138063

Evaluations for Submission to ENDF/B-VIII.1

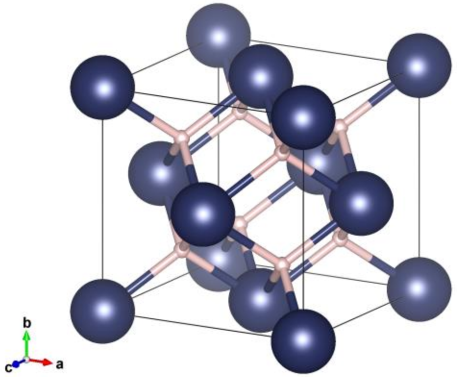
- Yttrium Hydride (YH_2)*
- Zirconium Hydride (ZrH_x and ZrH_2)*
- Enriched Lithium Hydride/Deuteride (^7LiH, ^7LiD)
- Beryllium Hydride (BeH_2)
- Beryllium Carbide (Be_2C)
- Zirconium Carbide (ZrC)
- Uranium Hydride ($H\text{-}UH_3$)**

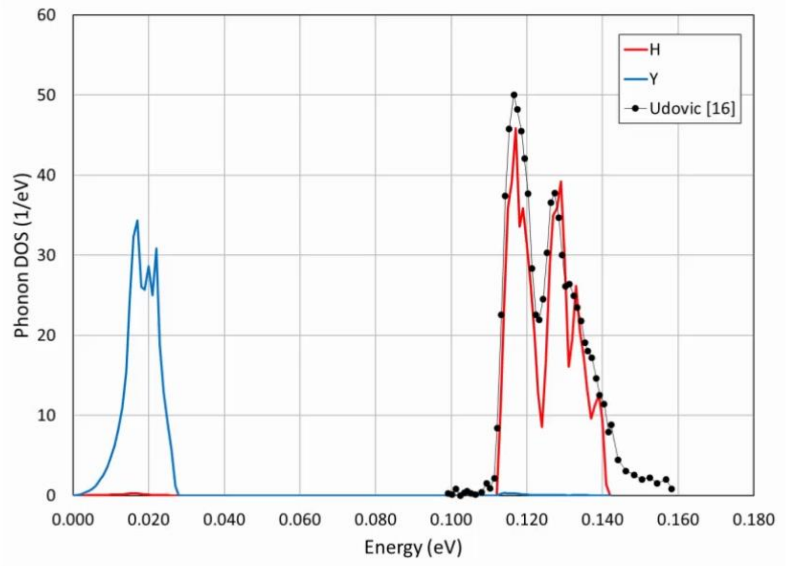
*Re-evaluation from ENDF/B-VIII.0

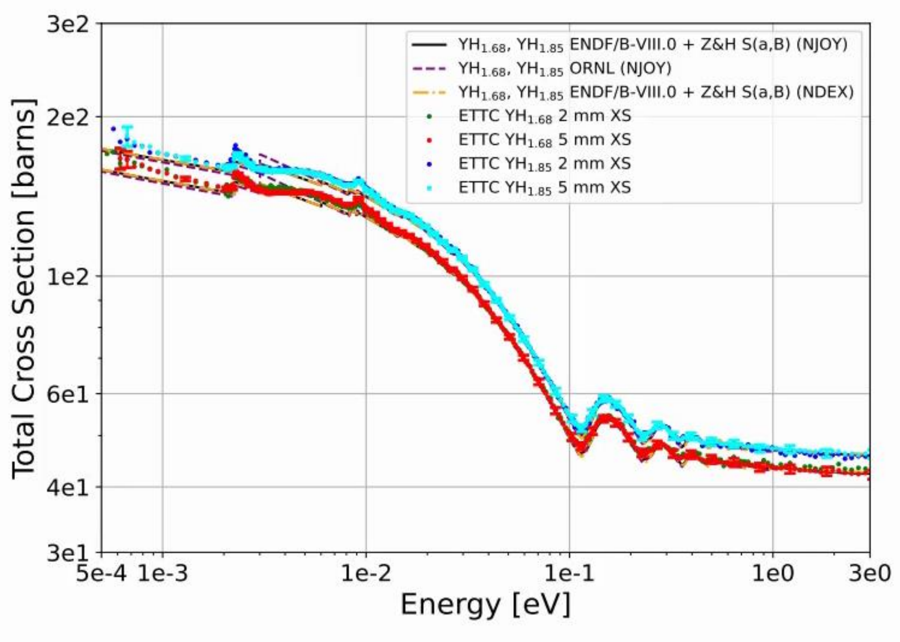
**Evaluated using LEAPR

Yttrium Hydride

- Naval Nuclear Laboratory evaluation included in ENDF/B-VIII.0
- Phonon DOS derived from AILD
  - H(YH_2) consistent with INS
  - Quantum oscillator
- Revised evaluation includes coherent elastic for Y(YH_x)
- Integrated cross section verified against recent transmission measurements
  - Bragg edges







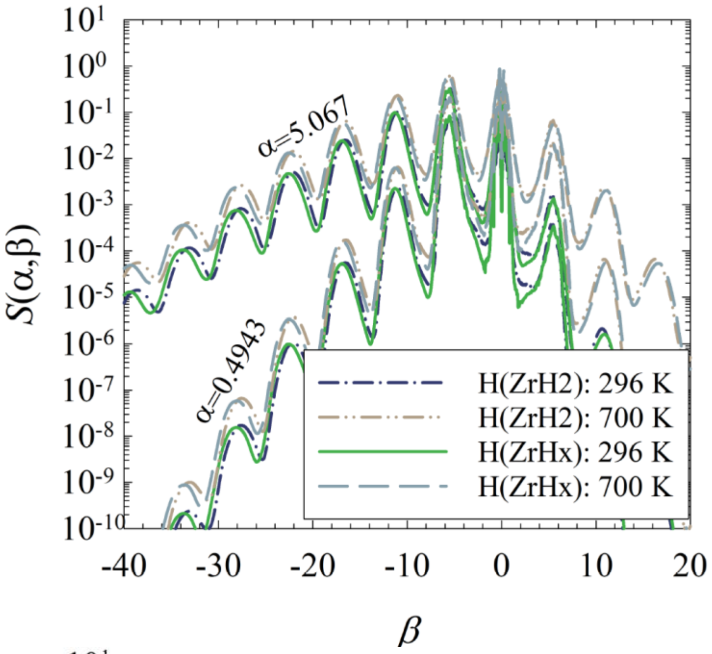
M.L. Zerkle, J.C. Holmes, J.L. Wormald, *EPJ Web of Conf.* **247**, 09015 (2021) https://doi.org/10.1051/epjconf/202124709015

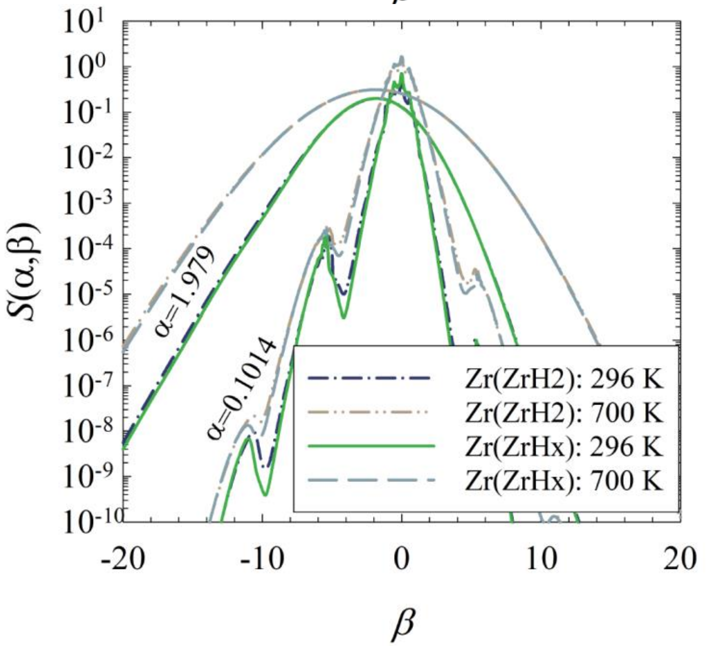
D. Fritz et al., *Ann. Nucl. Energy* **181**, 109475 (2022) https://doi.org/10.1016/j.anucene.2022.109475

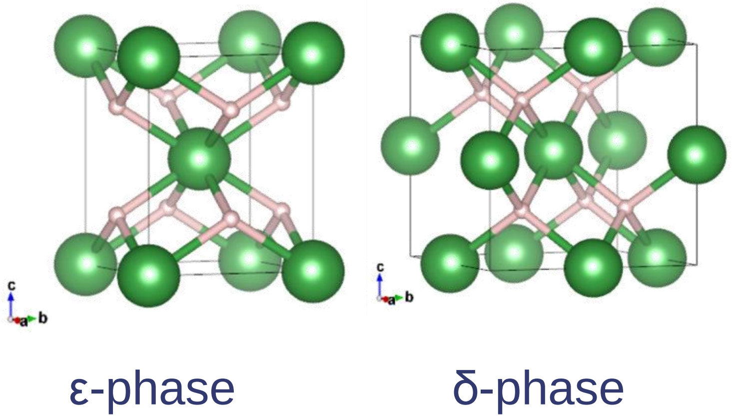
Zirconium Hydride

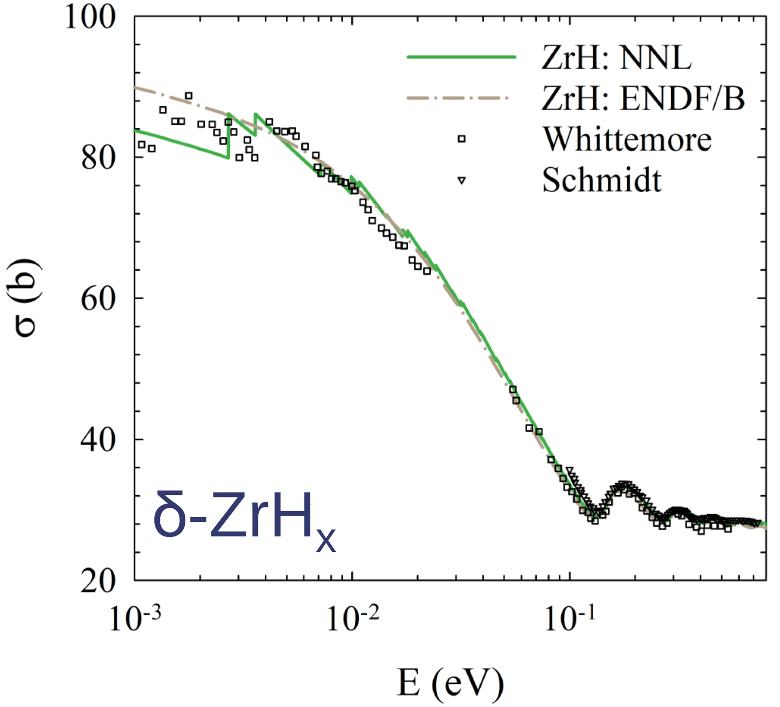
- Hybrid AIMD and AILD phonons
  - Quantum oscillator
  - Phonons DOS consistent with INS
- TSLs for δ-phase and ε-phase
  - Crystal structure on elastic scattering of Zr(ZrH$_x$)
    - ENDF/B-VIII.0 ZrH TSLs neglects crystal structure
    - Submission to include disordered alloy for Zr
  - ENDF/B-VIII.0 ZrH TSLs do not distinguish phase
- Preliminary TSL testing with critical mass and associated thermal flux
  - Less than 1% change in critical mass from ENDF/B-VIII.0 for HEU

J.L. Wormald, J.C. Holmes, and M.L. Zerkle, *JNE*, **2**,102 (2021) https://doi.org/10.3390/jne2020011





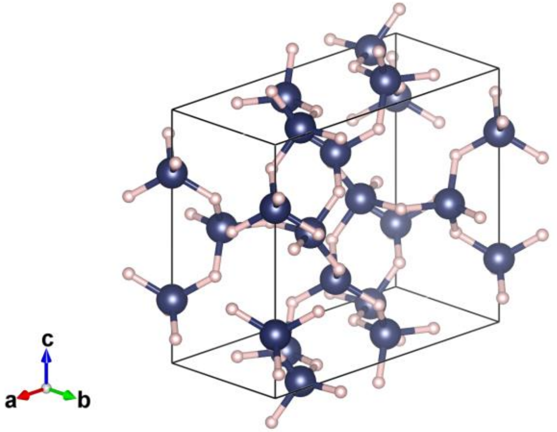


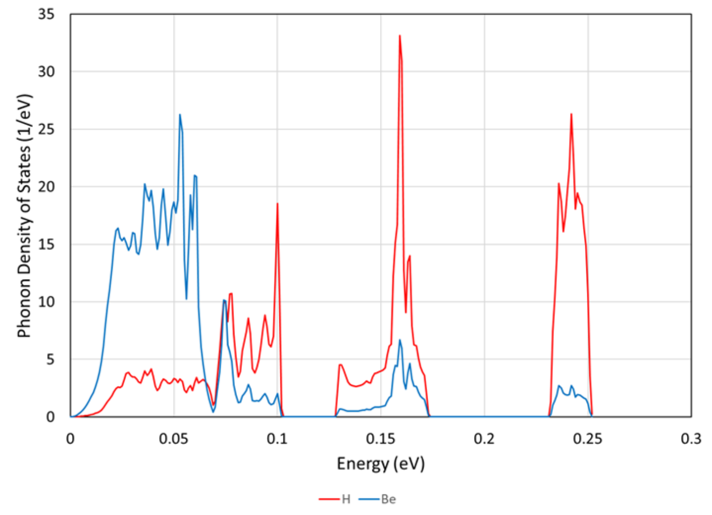


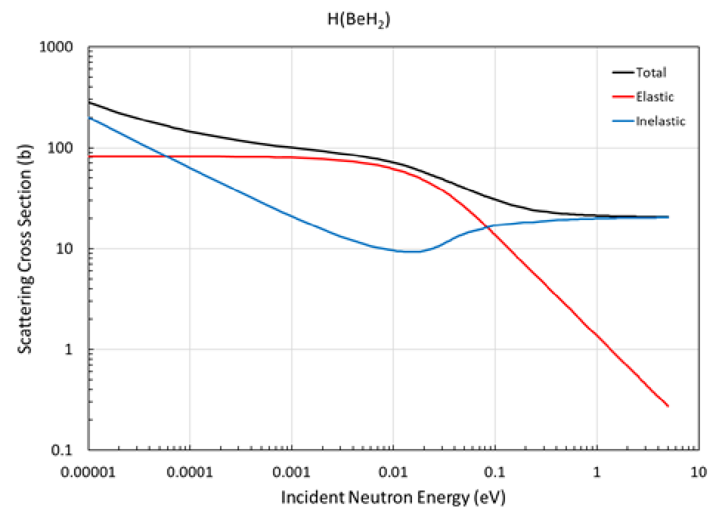
Beryllium Hydride

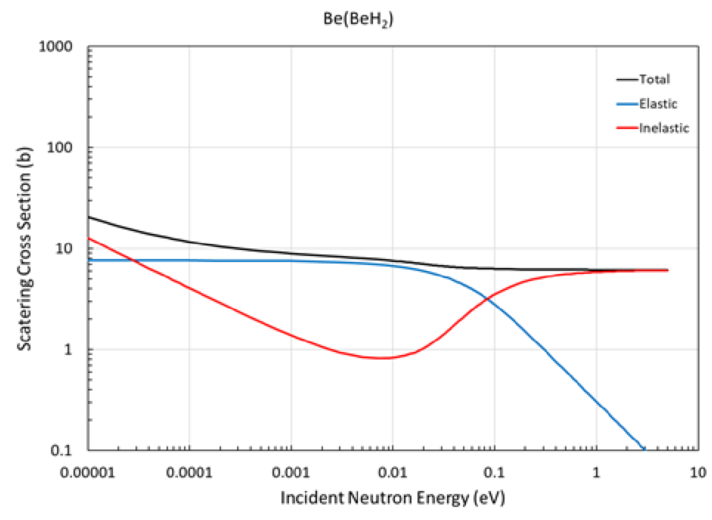
- TSLs for H(BeH_2) & Be(BeH_2) based on incoherent approximation
- PDOS from AILD calculations
  - Bending & stretching modes consistent with INS measurements for amorphous BeH_2
- Revision for coherent elastic will be considered

M.L. Zerkle, J.L. Wormald, J.C. Holmes, *NCSD-2022*, Anaheim CA (2022)

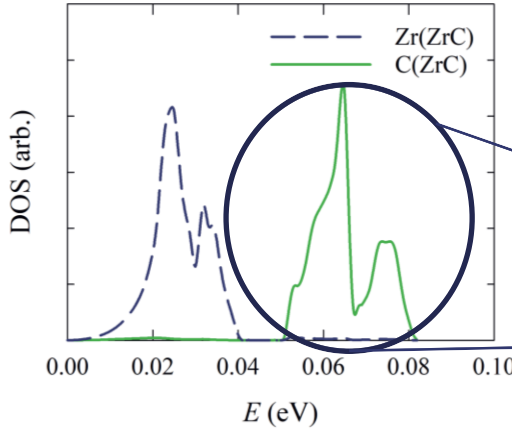


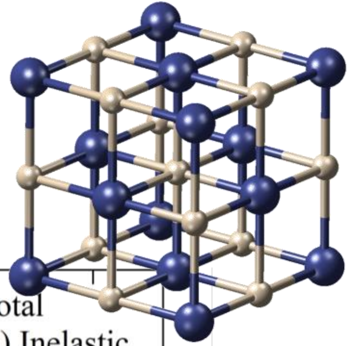


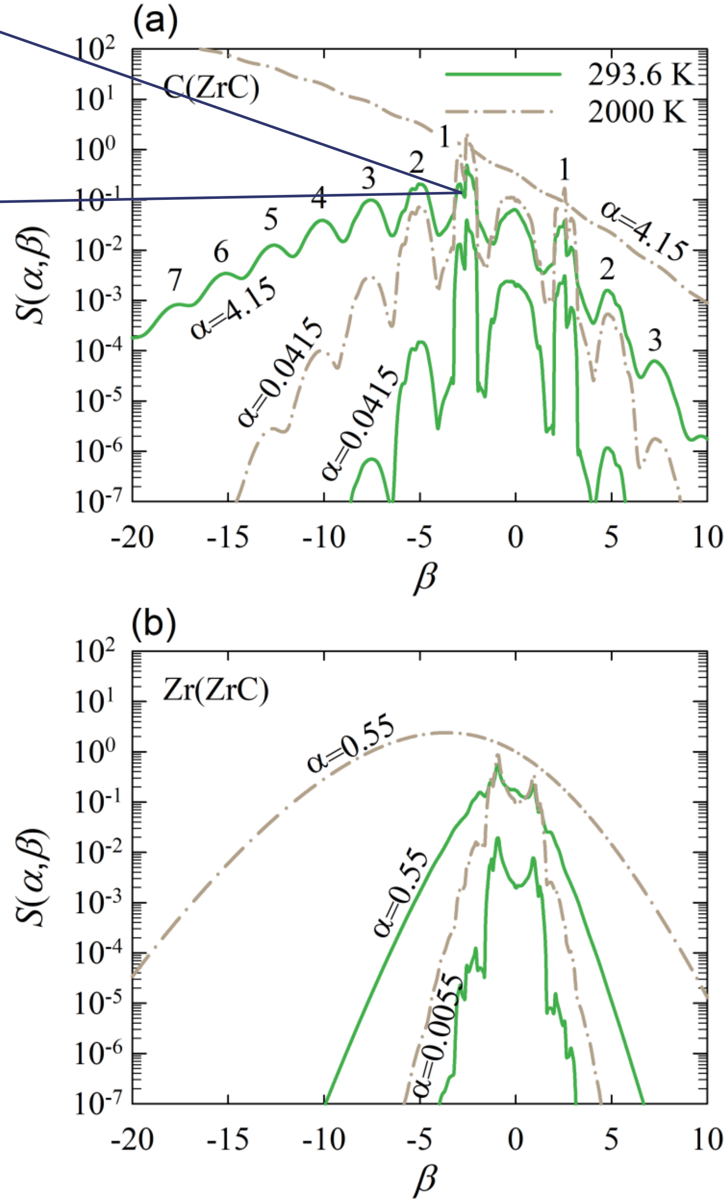


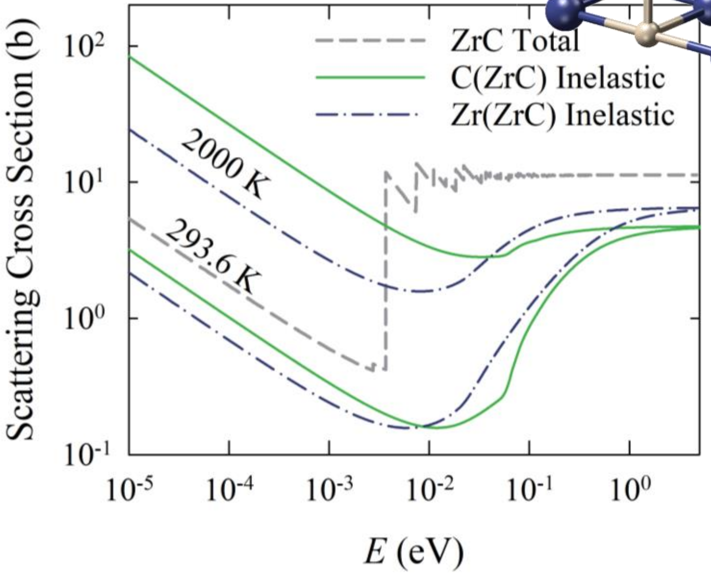


Zirconium Carbide

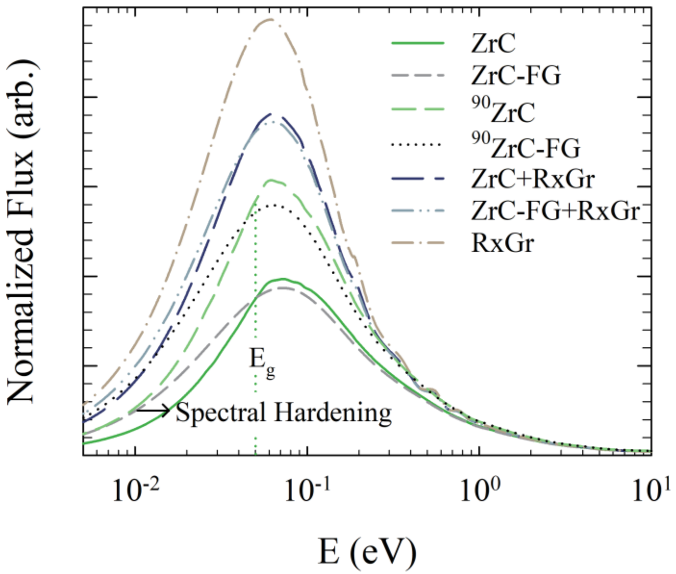








- AILD phonons
  - Phonon dispersion consistent with INS
  - Phonon band gap
  - Quantum oscillator
- C(ZrC) and Zr(ZrC) evaluation:
  - Mixed elastic scattering for C and Zr
  - Disordered alloy for C and Zr
  - Default automatic grid in FLASSH
- Effects testing:
  - Critical mass, temperature feedback, flux



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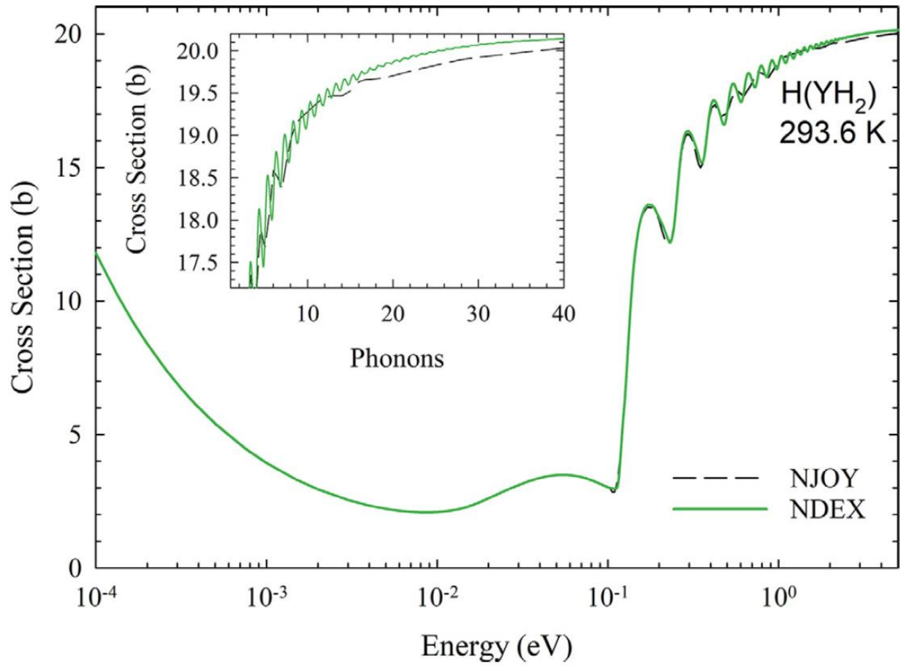
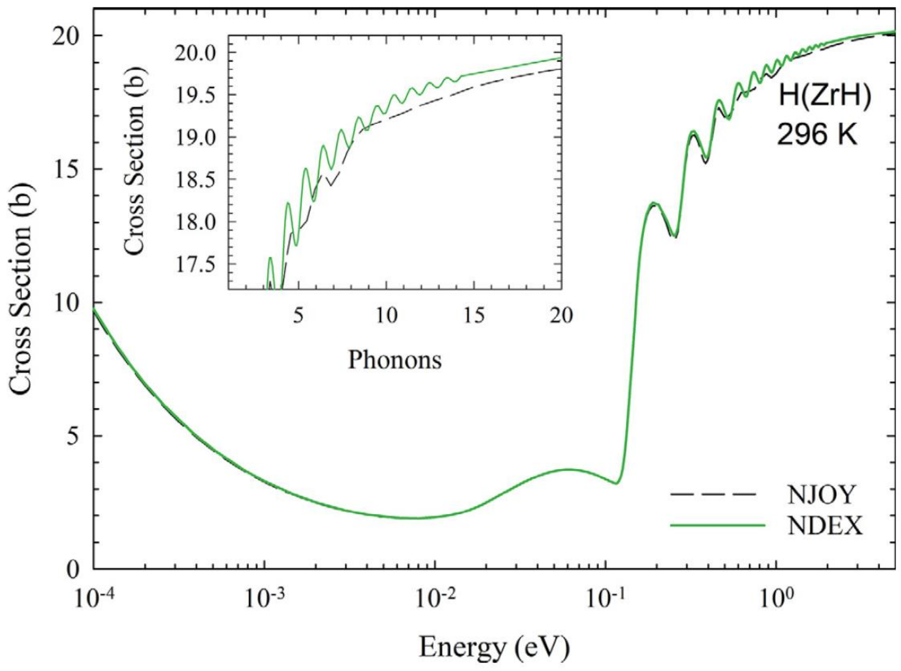
New Thermal Scattering Processing Methods

- Adaptive incident energy grids in NDEX improve numerical fidelity of metal hydride cross sections
  - NDEX vs NJOY2012
  - Uses β grid as starting incident energy grid to capture all cross section details of TSL
  - Differences in H(ZrH) cross sections associated with ≈ 60 pcm bias in ICSBEP TRIGA model (ICT-003) with MC21
  - J.L. Wormald, J.T. Thompson, T.H. Trumbull, *Annals of Nuclear Energy* **149** (2020) 107773 https://doi.org/10.1016/j.anucene.2020.107773

ENDF/B-VIII.0 TSL Evaluations





Summary

- Several evaluations for submission to ENDF/B-VIII.1
  - Sub-thermal transmission measurements for Be, YH_2, ZrC, and heavy paraffinic oils have been performed
  - Sub-thermal transmission measurements for ZrH_x under consideration
  - Follow-up ICSBEP analysis for ZrH_x
  - Quantum oscillator behavior identified to yield spectral effects
- New physics have been introduced to these evaluations
  - Elastic scattering extension
  - New *ab initio* methods for phonon generation
- New method to enhance cross section processing