Evaluation of the Thermal Scattering Law for Advanced Reactor Neutron Moderators and Reflectors

Ayman I. Hawari

Nuclear Reactor Program
Department of Nuclear Engineering
North Carolina State University
Raleigh, North Carolina, USA

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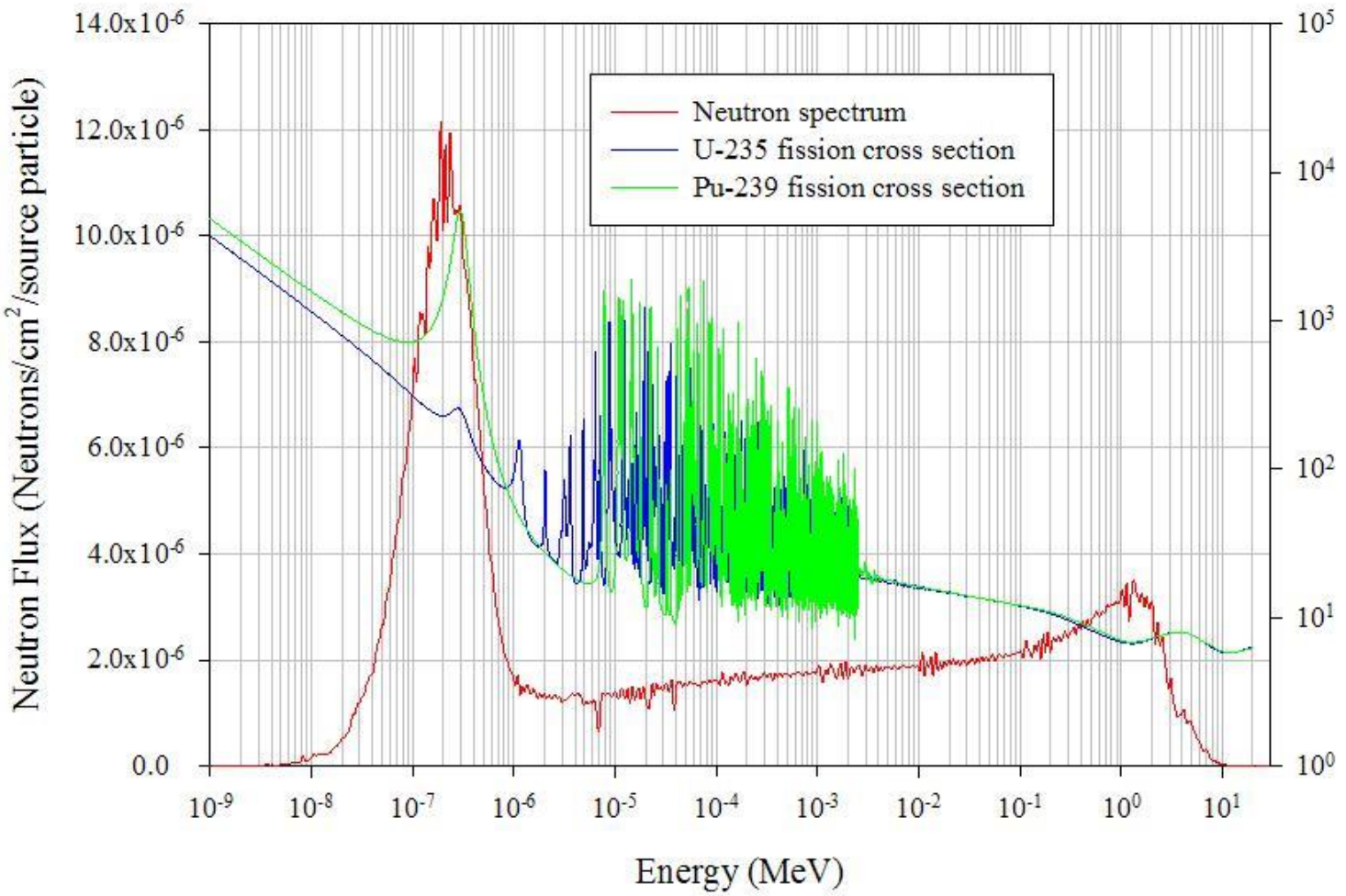
Motivation


Neutron spectrum
U-235 fission cross section
Pu-239 fission cross section
Neutron Flux (Neutrons/cm^2/source particle)
14.0x10^{-6}
12.0x10^{-6}
10.0x10^{-6}
8.0x10^{-6}
6.0x10^{-6}
4.0x10^{-6}
2.0x10^{-6}
0.0
10^5
10^4
10^3
10^2
10^1
10^0
10^{-9} 10^{-8} 10^{-7} 10^{-6} 10^{-5} 10^{-4} 10^{-3} 10^{-2} 10^{-1} 10^0 10^1
Energy (MeV)

Neutron Thermalization

Using first Born approximation combined with Fermi pseudopotential, it can be shown that the double differential scattering cross section has the form

$$\frac{d^2\sigma}{d\Omega dE'} = \frac{1}{4\pi}\sqrt{\frac{E'}{E}}\left\{\sigma_{coh}S(\vec{\kappa},\omega) + \sigma_{incoh}S_s(\vec{\kappa},\omega)\right\}$$

The scattering law $S(\vec{\kappa},\omega)$ is composed of two parts

$$S(\vec{\kappa},\omega) = S_s(\vec{\kappa},\omega) + S_d(\vec{\kappa},\omega)$$

Van Hove's space-time formulation

$$I(\vec{\kappa},t) = \int G(\vec{r},t)\exp(i\vec{\kappa}\cdot\vec{r})d\vec{r}$$

$$S(\vec{\kappa},\omega) = \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} G(\vec{r},t)e^{i(\vec{\kappa}\cdot\vec{r}-\omega t)}d\vec{r}dt$$

where $G(\vec{r},t)$ is the *dynamic pair correlation function* and can be expressed in terms of time dependent atomic positions.

Since 1960s
GASKET
NJOY/LEAPR
INCOHERENT
APPROXIMATION

$$S_s(\alpha,\beta) = k_B T \cdot S_s(\vec{\kappa},\omega)$$

$$\left.\frac{d^2\sigma}{d\Omega dE'}\right|_{inelastic} = \frac{\sigma}{2k_B T}\sqrt{\frac{E'}{E}}S_s(\alpha,\beta)$$

$\beta = \frac{E - E'}{k_B T}$ Energy transfer

$\alpha = \frac{(E + E' - 2\sqrt{EE'}\cos\theta)}{k_B T}$ Momentum transfer

The scattering law (TSL) is the Fourier transform of a Gaussian correlation function

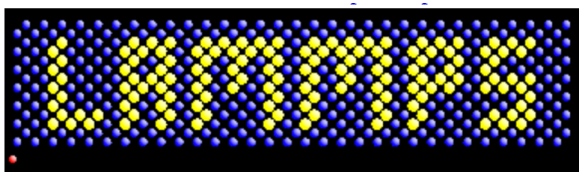
$$S_s(\alpha,\beta) = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{-i\beta t} e^{-\gamma(t)} dt$$

$$\gamma(t) = \frac{\alpha}{2}\int_{-\infty}^{\infty} \frac{\rho(\beta)}{\beta \sinh(\beta/2)}\left[1 - e^{-i\beta t}\right] e^{\beta/2} d\beta$$

$\rho(\beta)$ – density of states (e.g., phonon frequency distribution)

Thermal Scattering Law Analysis

- Key development in the last 20 years is the use of atomistic simulations methods to support the evaluation process
  - Produce data necessary to calculate the TSL including
    - DOS for evaluation of TSL
    - Direct access to TSL using correlation analysis



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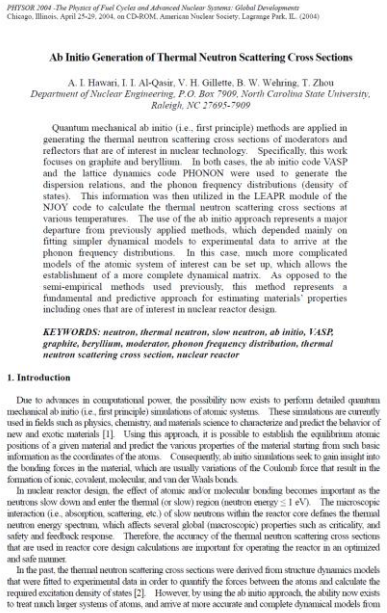

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Ab Initio Generation of Thermal Neutron Scattering Cross Sections

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Department of Nuclear Engineering, P.O. Box 7909, North Carolina State University, Raleigh, NC 27695-7909

Quantum mechanical ab initio (i.e., first principle) methods are applied in generating the thermal neutron scattering cross sections of moderators and reflectors that are of interest in nuclear technology. Specifically, this work focuses on graphite and beryllium. In both cases, the ab initio code VASP and the lattice dynamics code PHONON were used to generate the dispersion relations, and the phonon frequency distributions (density of states). This information was then utilized in the LEAPR module of the NJOY code to calculate the thermal neutron scattering cross sections at various temperatures. The use of the ab initio approach represents a major departure from previously applied methods, which depended mainly on fitting simpler dynamical models to experimental data to arrive at the phonon frequency distributions. In this case, much more complicated models of the atomic system of interest can be set up, which allows the establishment of a more complete dynamical matrix. As opposed to the semi-empirical methods used previously, this method represents a fundamental and predictive approach for estimating materials' properties including ones that are of interest in nuclear reactor design.

KEYWORDS: neutron, thermal neutron, slow neutron, ab initio, VASP, graphite, beryllium, moderator, phonon frequency distribution, thermal neutron scattering cross section, nuclear reactor

1. Introduction

Due to advances in computational power, the possibility now exists to perform detailed quantum mechanical ab initio (i.e., first principle) simulations of atomic systems. These simulations are currently used in fields such as physics, chemistry, and materials science to characterize and predict the behavior of new and exotic materials [1]. Using this approach, it is possible to establish the equilibrium atomic positions of a given material and predict the various properties of the material starting from such basic information as the coordinates of the atoms. Consequently, ab initio simulations seek to gain insight into the bonding forces in the material, which are usually variations of the Coulomb force that result in the formation of ionic, covalent, molecular, and van der Waals bonds.

In nuclear reactor design, the effect of atomic and/or molecular bonding becomes important as the neutrons slow down and enter the thermal (or slow) region (neutron energy ≤ 1 eV). The microscopic interaction (i.e., absorption, scattering, etc.) of slow neutrons within the reactor core defines the thermal neutron energy spectrum, which affects several global (macroscopic) properties such as criticality, and safety and feedback response. Therefore, the accuracy of the thermal neutron scattering cross sections that are used in reactor core design calculations are important for operating the reactor in an optimized and safe manner.

In the past, the thermal neutron scattering cross sections were derived from structure dynamics models that were fitted to experimental data in order to quantify the forces between the atoms and calculate the required excitation density of states [2]. However, by using the ab initio approach, the ability now exists to treat much larger systems of atoms, and arrive at more accurate and complete dynamical models from

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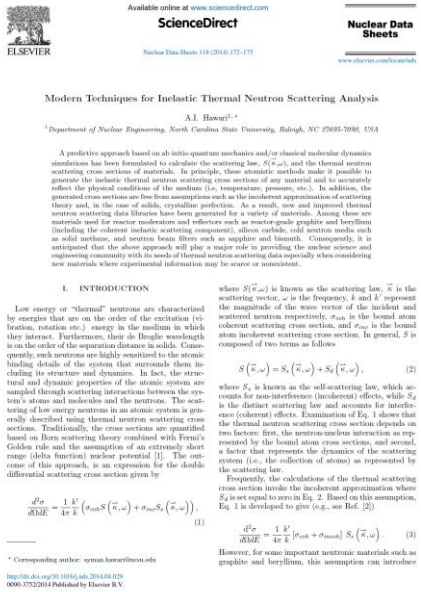

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Modern Techniques for Inelastic Thermal Neutron Scattering Analysis

A.I. Hawari[1,*]
[1]*Department of Nuclear Engineering, North Carolina State University, Raleigh, NC 27695-7909, USA*

A predictive approach based on ab initio quantum mechanics and/or classical molecular dynamics simulations has been formulated to calculate the scattering law, $S(\vec{\kappa},\omega)$, and the thermal neutron scattering cross sections of materials. In principle, these atomistic methods make it possible to generate the inelastic thermal neutron scattering cross sections of any material and to accurately reflect the physical conditions of the medium (i.e., temperature, pressure, etc.). In addition, the generated cross sections are free from assumptions such as the incoherent approximation of scattering theory and, in the case of solids, crystalline perfection. As a result, new and improved thermal neutron scattering data libraries have been generated for a variety of materials. Among these are materials used for reactor moderators and reflectors such as reactor-grade graphite and beryllium (including the coherent inelastic scattering component), silicon carbide, cold neutron media such as solid methane, and neutron beam filters such as sapphire and bismuth. Consequently, it is anticipated that the above approach will play a major role in providing the nuclear science and engineering community with its needs of thermal neutron scattering data especially when considering new materials where experimental information may be scarce or nonexistent.

1. INTRODUCTION

Low energy or "thermal" neutrons are characterized by energies that are on the order of the excitation (vibration, rotation etc.) energy in the medium in which they interact. Furthermore, their de Broglie wavelength is on the order of the separation distance in solids. Consequently, such neutrons are highly sensitized to the atomic binding details of the system that surrounds them including its structure and dynamics. In fact, the structural and dynamic properties of the atomic system are sampled through scattering interactions between the system's atoms and molecules and the neutrons. The scattering of low energy neutrons in an atomic system is generally described using thermal neutron scattering cross sections. Traditionally, the cross sections are quantified based on Born scattering theory combined with Fermi's Golden rule and the assumption of an extremely short range (delta function) nuclear potential [1]. The outcome of this approach, is an expression for the double differential scattering cross section given by

$$\frac{d^2\sigma}{d\Omega dE} = \frac{1}{4\pi}\frac{k'}{k}\left(\sigma_{coh}S\left(\vec{\kappa},\omega\right)+\sigma_{inc}S_s\left(\vec{\kappa},\omega\right)\right), \quad (1)$$

where $S(\vec{\kappa},\omega)$ is known as the scattering law, $\vec{\kappa}$ is the scattering vector, ω is the frequency, k and k' represent the magnitude of the wave vector of the incident and scattered neutron respectively, σ_{coh} is the bound atom coherent scattering cross section, and σ_{inc} is the bound atom incoherent scattering cross section. In general, S is composed of two terms as follows

$$S\left(\vec{\kappa},\omega\right) = S_s\left(\vec{\kappa},\omega\right) + S_d\left(\vec{\kappa},\omega\right), \quad (2)$$

where S_s is known as the self-scattering law, which accounts for non-interference (incoherent) effects, while S_d is the distinct scattering law and accounts for interference (coherent) effects. Examination of Eq. 1 shows that the thermal neutron scattering cross section depends on two factors: first, the neutron-nucleus interaction as represented by the bound atom cross sections, and second, a factor that represents the dynamics of the scattering system (i.e., the collection of atoms) as represented by the scattering law.

Frequently, the calculations of the thermal scattering cross section invoke the incoherent approximation where S_d is set equal to zero in Eq. 2. Based on this assumption, Eq. 1 is developed to give (e.g., see Ref. [2])

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* Corresponding author: ayman.hawari@ncsu.edu

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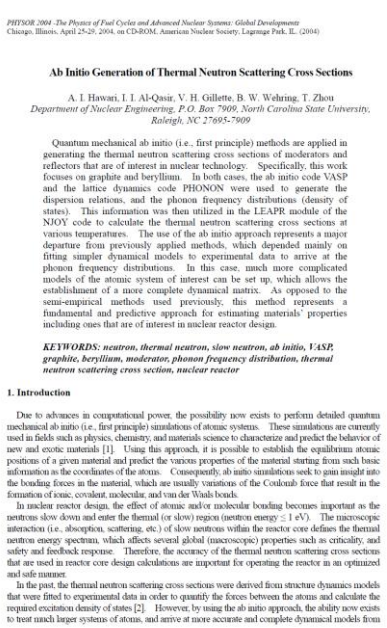

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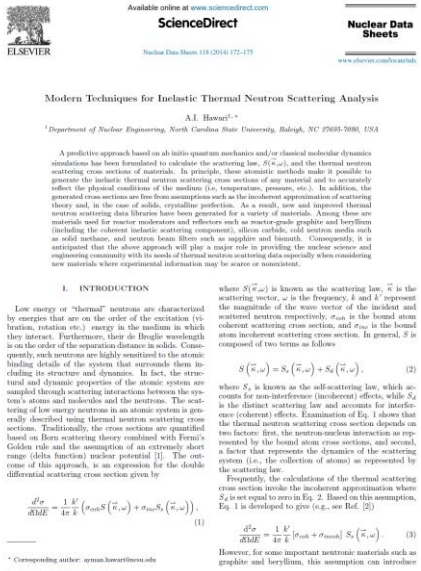

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D. A. Brown,[1] M. B. Chadwick,[2,*] R. Capote,[3] A. C. Kahler,[2] A. Trkov,[3] M. W. Herman,[1] A. A. Sonzogni,[1] Y. Danon,[4] A. D. Carlson,[5] M. Dunn,[6] D. L. Smith,[7] G. M. Hale,[2] G. Arbanas,[8] R. Arcilla,[1] C.R. Bates,[2] B. Beck,[9] B. Becker,[10] F. Brown,[2] R. J. Casperson,[2] J. Conlin,[2] D. E. Cullen,[9] M.-A. Descalle,[6] R. Firestone,[11] T. Gaines,[12] K. H. Guber,[8] A. I. Hawari,[13] J. Holmes,[14] T. D. Johnson,[1] T. Kawano,[2] B. C. Kiedrowski,[15] A. J. Koning,[3] S. Kopecky,[16] L. Leal,[17] J. P. Lestone,[2] C. Lubitz,[18] J. I. Márquez Damián,[19] C. M. Mattoon,[8] E. A. McCutchan,[1] S. Mughabghab,[1] P. Navratil,[20] D. Neudecker,[2] G. P. A. Nobre,[1] G. Noguere,[21] M. Paris,[2] M. T. Pigni,[6] A. J. Plompen,[16] B. Pritychenko,[1] V. G. Pronyaev,[22] D. Roubtsov,[23] D. Rochman,[24] P. Romano,[7] P. Schillebeeckx,[16] S. Simakov,[25] M. Sin,[26] I. Sirakov,[27] B. Sleaford,[9] V. Sobes,[6] E. S. Soukhovitskii,[28] I. Stetcu,[2] P. Talou,[2] I. Thompson,[2] S. van der Marck,[29] L. Welser-Sherrill,[2] D. Wiarda,[8] M. White,[2] J. L. Wormald,[15] R. Q. Wright,[8] M. Zerkle,[14] G. Zerovnik,[16] and Y. Zhu[15]

[1]*Brookhaven National Laboratory, Upton, NY 11973-5000, USA*
[2]*Los Alamos National Laboratory, Los Alamos, NM 87545, USA*
[3]*International Atomic Energy Agency, PO Box 100, A-1400 Vienna, Austria*
[4]*Rensselaer Polytechnic Institute, Troy, NY 12180, USA*
[5]*National Institute of Standards and Technology, Gaithersburg, MD 20899-8463, USA*
[6]*Spectra Tech, Inc., Oak Ridge, TN 37830, USA*
[7]*Argonne National Laboratory, Argonne, IL 60439-4842, USA*
[8]*Oak Ridge National Laboratory, Oak Ridge, TN 37831-6171, USA*
[9]*Lawrence Livermore National Laboratory, Livermore, CA 94551-0808, USA*
[10]*Gesellschaft für Anlagen und Reaktorsicherheit, Schwertnergasse 1, D-50667 Köln, Germany*
[11]*Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA*
[12]*AWE plc, Reading RG7 4PR, United Kingdom*
[13]*North Carolina State University, Raleigh, NC 27695, USA*
[14]*Naval Nuclear Laboratory, West Mifflin, PA 15122, USA*
[15]*University of Michigan, Ann Arbor, MI 48109, USA*
[16]*EC-JRC, B-2440 Geel, Belgium*
[17]*Institut de Radioprotection et de Sûreté Nucléaire, 92262 Fontenay aux Roses, Cedex, France*
[18]*Naval Nuclear Laboratory, Niskayuna, NY 12309, USA*
[19]*Centro Atómico Bariloche, S. C. de Bariloche, Argentina*
[20]*TRIUMF, Vancouver, BC V6T 2A3, Canada*
[21]*CEA, DEN, DER, SPRC, Cadarache, 13108 Saint-Paul-lès-Durance, France*
[22]*IH, Atomstandart at SC Rosatom, Moscow, Russian Federation*
[23]*Canadian Nuclear Laboratories, Chalk River, Ontario, Canada*
[24]*Paul Scherrer Institut, 5232 Villigen, Switzerland*
[25]*Karlsruhe Institute of Technology, Hermann-von-Helmholtz-Platz, 1 76344 Eggenstein-Leopoldshafen, Germany*
[26]*University of Bucharest, Bucharest-Magurele, RO-077125, Romania*
[27]*Institute for Nuclear Research and Nuclear Energy, BAS, BG-1784 Sofia, Bulgaria*
[28]*Joint Institute for Energy and Nuclear Research, Minsk, Belarus*
[29]*NRG, Westerduinweg 3, 1755 LE Petten, The Netherlands*
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We describe the new ENDF/B-VIII.0 evaluated nuclear reaction data library. ENDF/B-VIII.0 fully incorporates the new IAEA standards, includes improved thermal neutron scattering data and uses new evaluated data from the CIELO project for neutron reactions on ^{1}H, ^{16}O, ^{56}Fe, ^{235}U, ^{238}U and ^{239}Pu described in companion papers in the present issue of *Nuclear Data Sheets*. The evaluations benefit from recent experimental data obtained in the U.S. and Europe, and improvements in theory and simulation. Notable advances include updated evaluated data for light nuclei, structural materials, actinides, fission energy release, prompt fission neutron and γ-ray spectra, thermal neutron scattering data, and charged-particle reactions. Integral validation testing is shown for a wide range of criticality, reaction rate, and neutron transmission benchmarks. In general, integral validation performance of the library is improved relative to the previous ENDF/B-VII.1 library.

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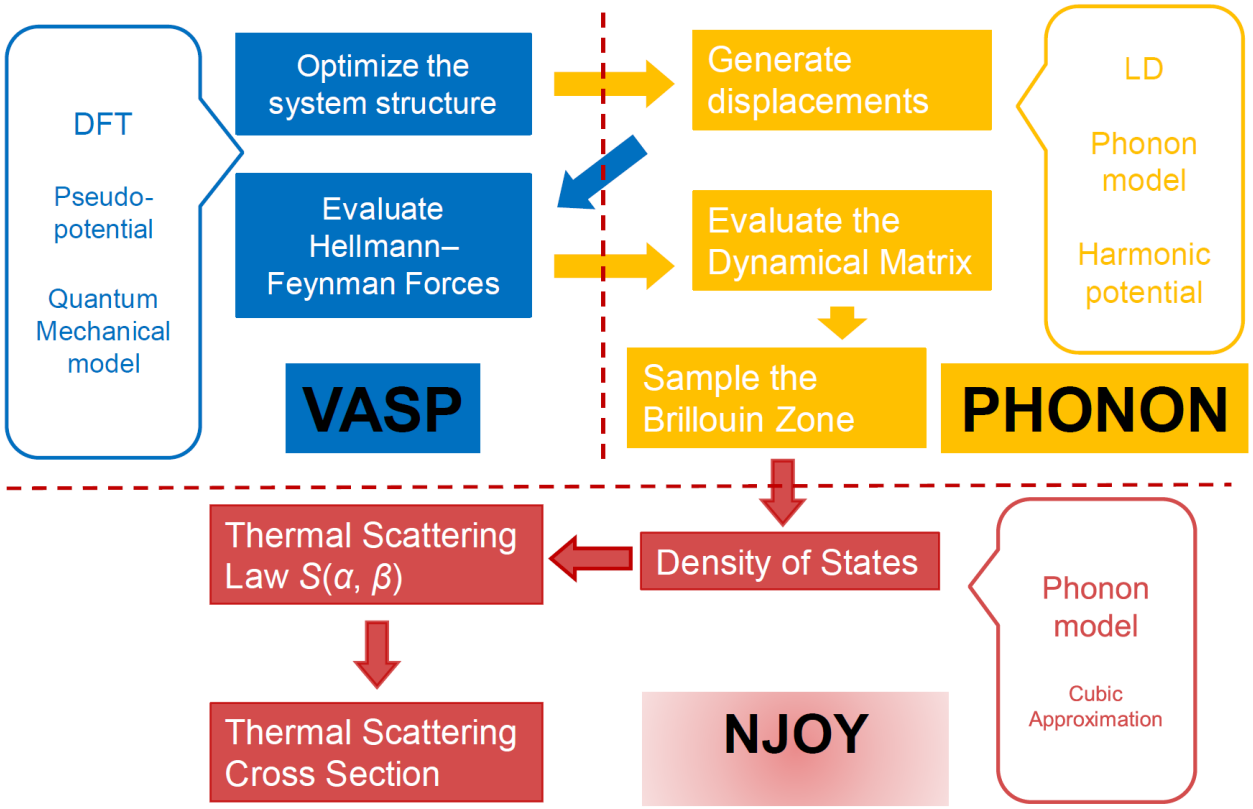
2000 - Present

Evaluation Approach

- Construct atomistic model of a material
- Verify ability of model to reproduce physical properties of the material (equilibrium conditions)
  - Density, thermal expansion, thermal conductivity,…
  - Ergodic behavior, correlations,…
- Generate input (DOS, …) for TSL calculations
- Calculate TSL and produce thermal scattering cross sections
  - Check consistency of results with computational assumptions/models
  - Compare to experimental data

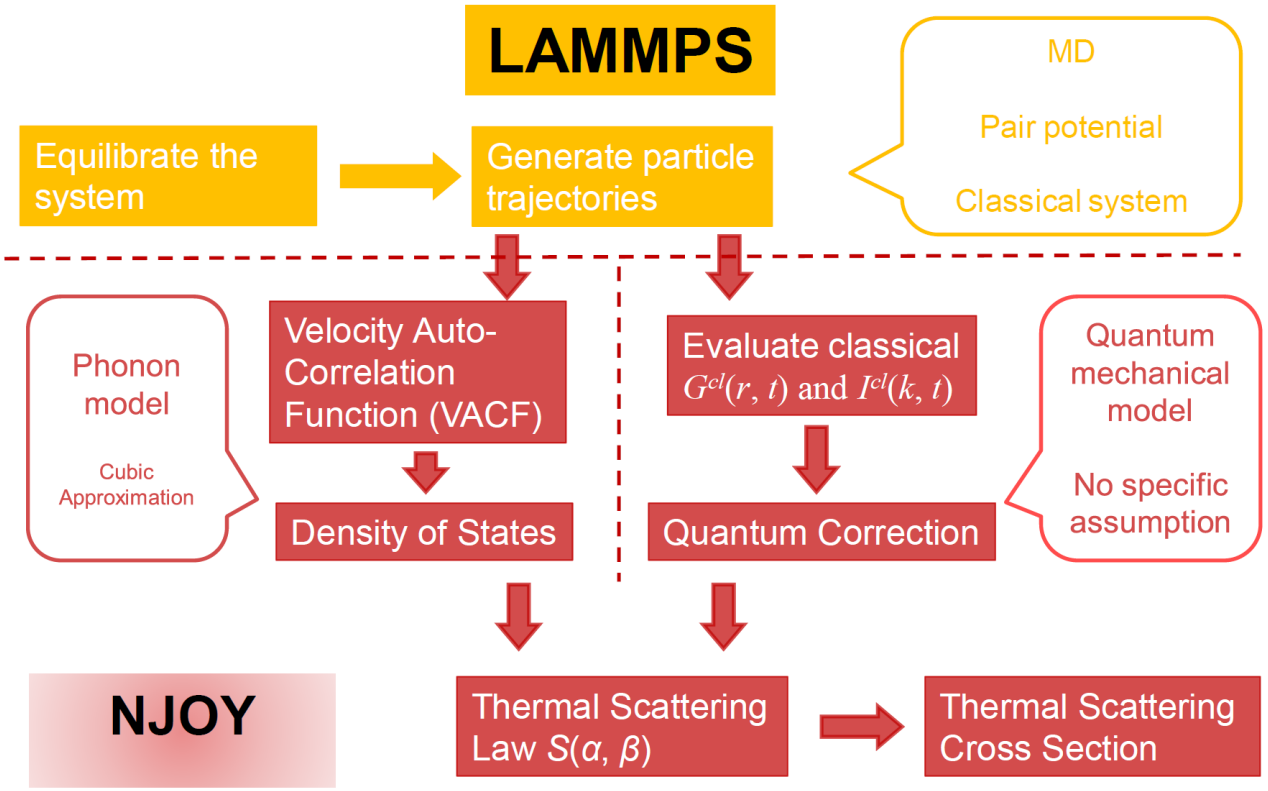
Thermal Scattering Cross-Sections

Evaluation DFT/LD



Thermal Scattering Cross-Sections

Evaluation MD/QM



ENDF/B-VIII TSL Evaluations

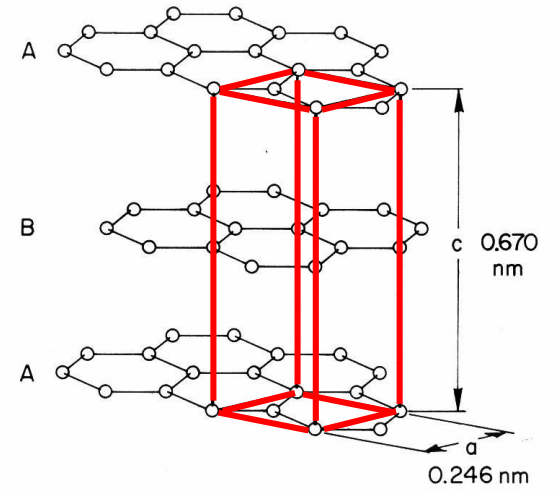
Material	ENDF Library Name	Evaluation Basis	Institution
Beryllium metal	tsl-Be-metal.endf	DFT/LD	NCSU
Beryllium oxide (beryllium)	tsl-BeinBeO.endf	DFT/LD	NCSU
Beryllium oxide (oxygen)	tsl-OinBeO.endf	DFT/LD	NCSU
Light water (hydrogen)	tsl-HinH2O.endf	MD	CAB
Light water ice (hydrogen)	tsl-HinIceIh.endf	DFT/LD	BAPL
Light water ice (oxygen)	tsl-OinIceIh.endf	DFT/LD	BAPL
Heavy water (deuterium)	tsl-DinD2O.endf	MD	CAB
Heavy water (oxygen)	tsl-OinD2O.endf	MD	CAB
Polymethyl Methacrylate (Lucite)	tsl-HinC5O2H8.endf	MD	NCSU
Polyethylene	tsl-HinCH2.endf	MD	NCSU
Crystalline graphite	tsl-graphite.endf	MD	NCSU
Reactor graphite (10% porosity)	tsl-reactor-graphite-10P.endf	MD	NCSU
Reactor graphite (30% porosity)	tsl-reactor-graphite-30P.endf	MD	NCSU
Silicon carbide (silicon)	tsl-CinSiC.endf	DFT/LD	NCSU
Silicon carbide (carbon)	tsl-SiinSiC.endf	DFT/LD	NCSU
Silicon dioxide (alpha phase)	tsl-SiO2-alpha.endf	DFT/LD	NCSU
Silicon dioxide (beta phase)	tsl-SiO2-beta.endf	DFT/LD	NCSU
Yttrium hydride (hydrogen)	tsl-HinYH2.endf	DFT/LD	BAPL
Yttrium hydride (yttrium)	tsl-YinYH2.endf	DFT/LD	BAPL
Uranium dioxide (oxygen)	tsl-OinUO2.endf	DFT/LD	NCSU
Uranium dioxide (uranium)	tsl-UinUO2.endf	DFT/LD	NCSU
Uranium nitride (nitrogen)	tsl-NinUN.endf	DFT/LD	NCSU
Uranium nitride (uranium)	tsl-UinUN.endf	DFT/LD	NCSU

ENDF/B-VIII TSL Evaluations

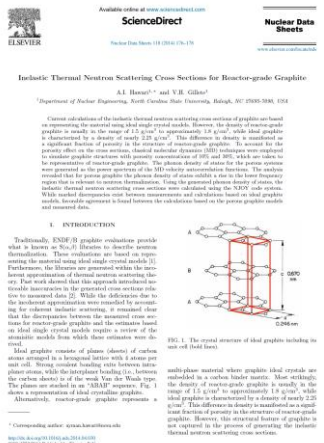
Material	ENDF Library Name	Evaluation Basis	Institution
Beryllium metal	tsl-Be-metal.endf	DFT/LD	NCSU
Beryllium oxide (beryllium)	tsl-BeinBeO.endf	DFT/LD	NCSU
Beryllium oxide (oxygen)	tsl-OinBeO.endf	DFT/LD	NCSU
Light water (hydrogen)	tsl-HinH2O.endf	MD	CAB
Light water ice (hydrogen)	tsl-HinIceIh.endf	DFT/LD	BAPL
Light water ice (oxygen)	tsl-OinIceIh.endf	DFT/LD	BAPL
Heavy water (deuterium)	tsl-DinD2O.endf	MD	CAB
Heavy water (oxygen)	tsl-OinD2O.endf	MD	CAB
Polymethyl Methacrylate (Lucite)	tsl-HinC5O2H8.endf	MD	NCSU
Polyethylene	tsl-HinCH2.endf	MD	NCSU
Crystalline graphite	tsl-graphite.endf	MD	NCSU
Reactor graphite (10% porosity)	tsl-reactor-graphite-10P.endf	MD	NCSU
Reactor graphite (30% porosity)	tsl-reactor-graphite-30P.endf	MD	NCSU
Silicon carbide (silicon)	tsl-CinSiC.endf	DFT/LD	NCSU
Silicon carbide (carbon)	tsl-SiinSiC.endf	DFT/LD	NCSU
Silicon dioxide (alpha phase)	tsl-SiO2-alpha.endf	DFT/LD	NCSU
Silicon dioxide (beta phase)	tsl-SiO2-beta.endf	DFT/LD	NCSU
Yttrium hydride (hydrogen)	tsl-HinYH2.endf	DFT/LD	BAPL
Yttrium hydride (yttrium)	tsl-YinYH2.endf	DFT/LD	BAPL
Uranium dioxide (oxygen)	tsl-OinUO2.endf	DFT/LD	NCSU
Uranium dioxide (uranium)	tsl-UinUO2.endf	DFT/LD	NCSU
Uranium nitride (nitrogen)	tsl-NinUN.endf	DFT/LD	NCSU
Uranium nitride (uranium)	tsl-UinUN.endf	DFT/LD	NCSU

Graphite

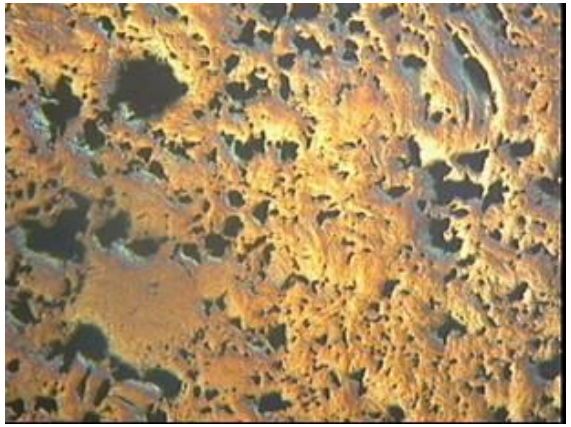
Ideal "crystalline" graphite consists of planes (sheets) of carbon atoms arranged in a hexagonal lattice. Covalent bonding exits between intraplaner atoms, while the interplaner bonding is of the weak Van der Waals type. The planes are stacked in an "abab" sequence.



- Hexagonal Structure
- 4 atoms per unit cell
- a = b = 2.46 Å
- c = 6.7 Å
- Density = 2.25 g/cm^3

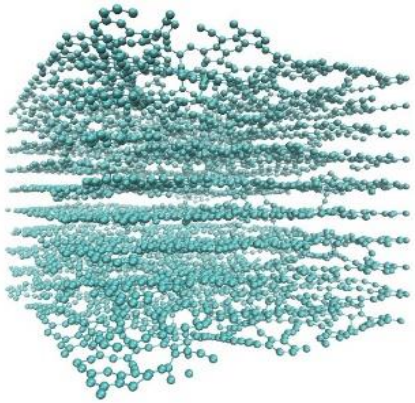


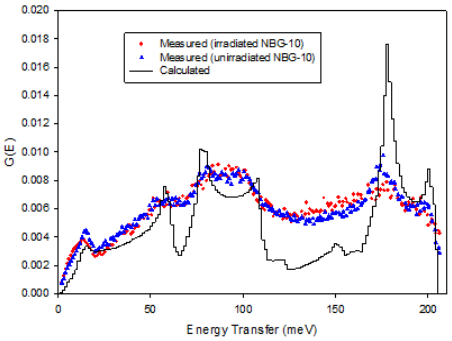
Reactor/Nuclear graphite consists of ideal graphite crystallites (randomly oriented) in a carbon binder. It is highly porous structure with porosity level ranging between 10% and 30%.

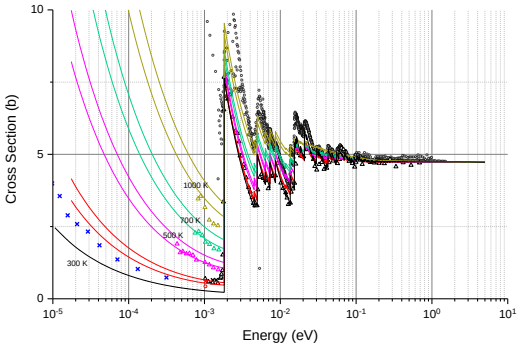


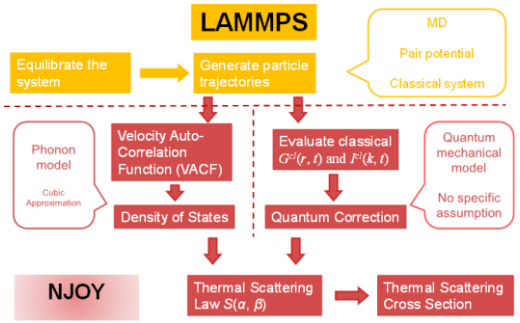
Nuclear Graphite (SEM at NCSU)
Density = 1.5 – 1.8 g/cm^3

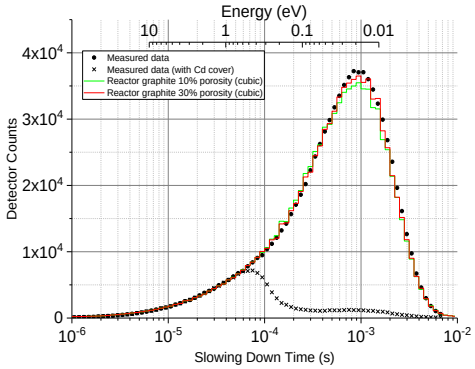
Reactor/Nuclear Graphite

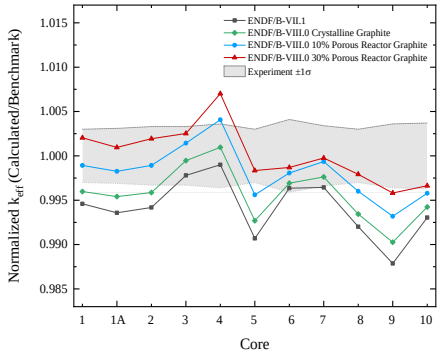








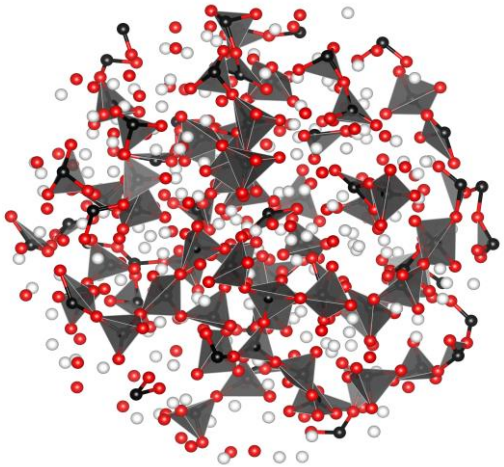


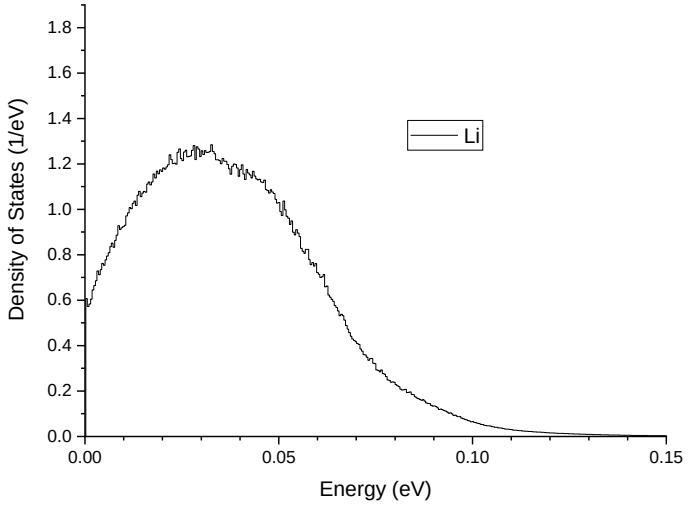


Evaluation

Measurements/Benchmarks

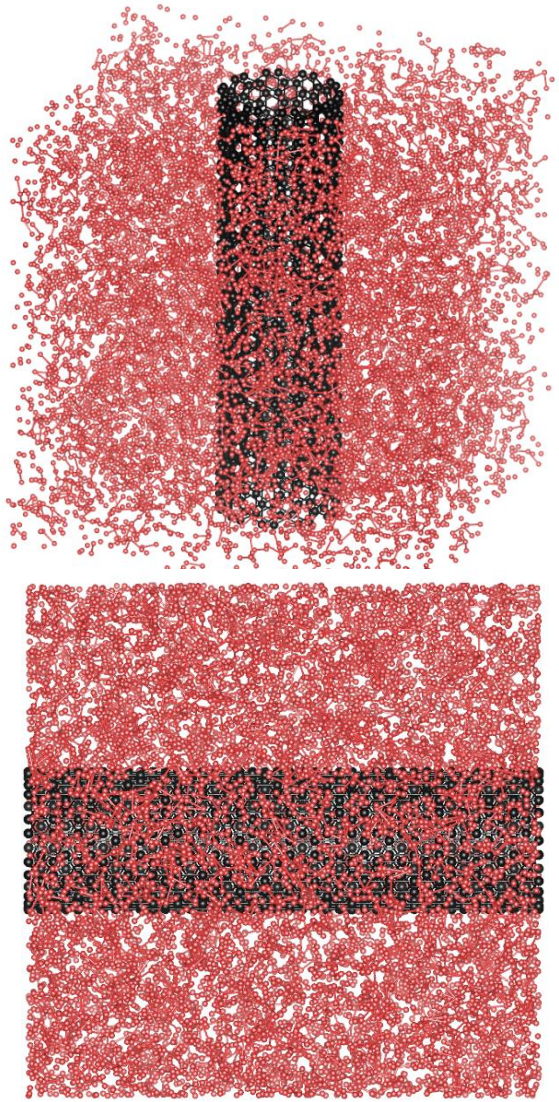
Liquid FLiBe





- Eutectic with a mixture of 2:1 ratio of LiF and BeF2
- Melting Point: 732K Boiling Point:1703K
- DFT and MD analysis (with QM corrections)
- TSL evaluation between 750K and 1500K

Carbon-Carbon Composite



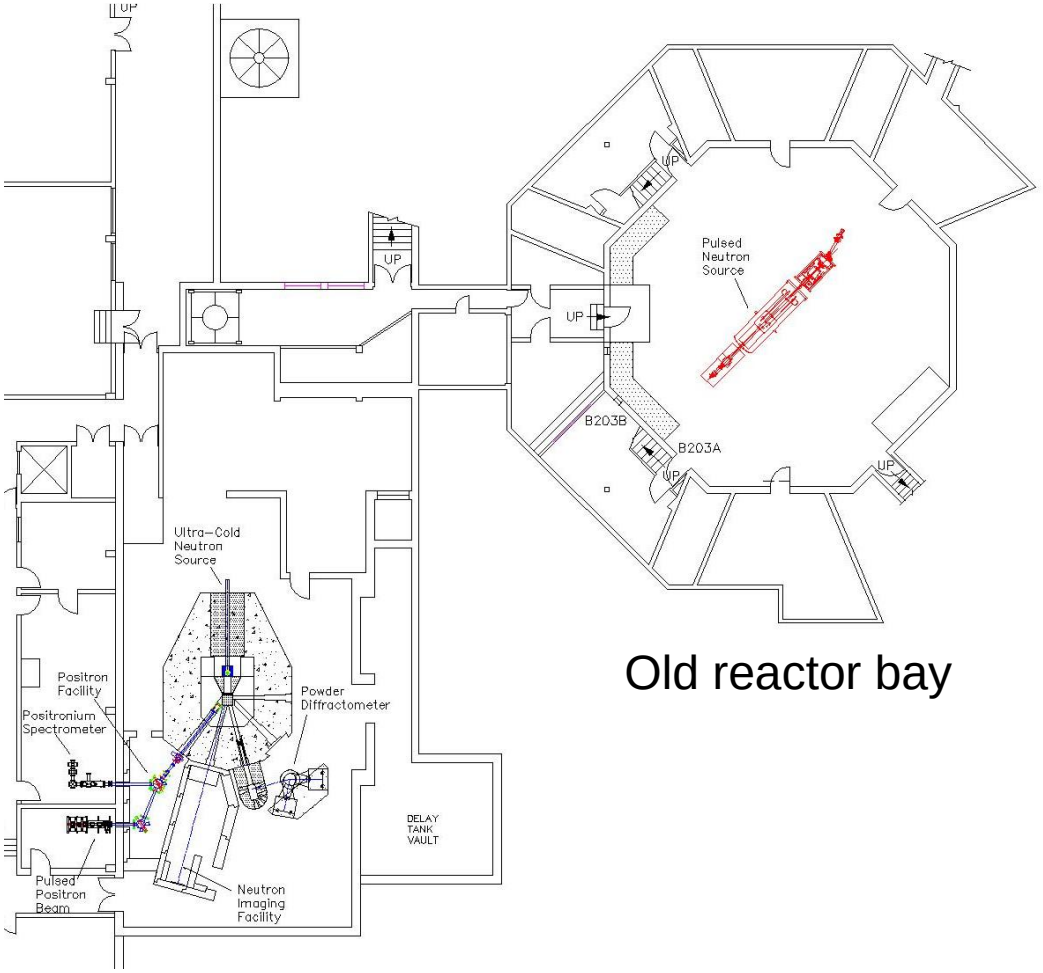
- Carbon fiber embedded in a carbon matrix.
- Density may vary in the range of 1.6 to 2.0 g/cm^3.
- MD analysis (with QM corrections)
- TSL evaluation

Current major facilities/capabilities

- Neutron powder diffraction
- Neutron imaging
- Intense positron beam
- Ultracold neutron source (under testing)
- Neutron activation analysis
- In-pool irradiation testing facilities

Current projects

- PULSTAR power upgrade 1-2 MW (licensing stage)
- Various instrument and facility upgrades
- Pulsed accelerator neutron source (under testing)
- Fuel loop for fission gas release studies



Old reactor bay

PULSTAR reactor bay

Current major facilities/capabilities

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- Neutron imaging
- **Intense positron beam**
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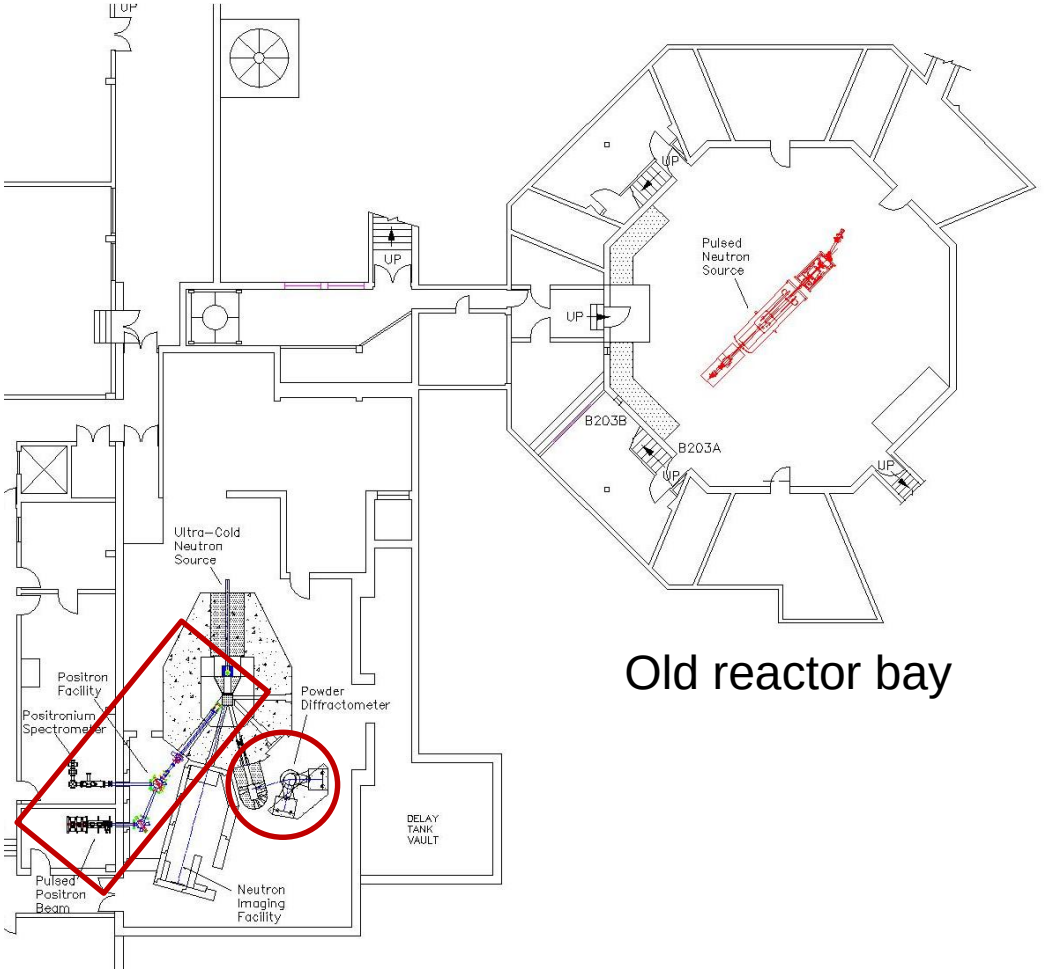

Old reactor bay

PULSTAR reactor bay

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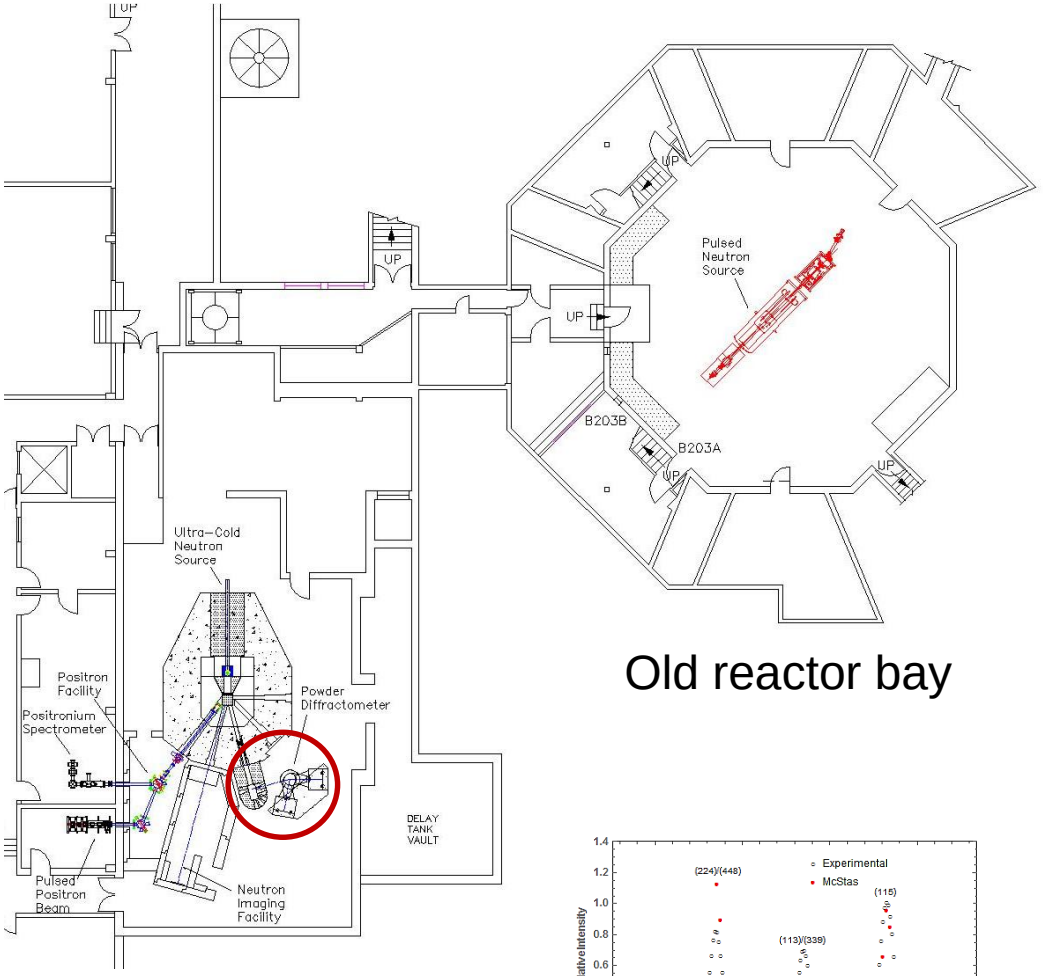


Old reactor bay

PULSTAR reactor bay

Neutron Thermalization

Using first Born approximation combined with Fermi pseudopotential, it can be shown that the double differential scattering cross section has the form

$$\frac{d^2\sigma}{d\Omega dE'} = \frac{1}{4\pi}\sqrt{\frac{E'}{E}}\left\{\sigma_{coh}S(\vec{\kappa},\omega) + \sigma_{incoh}S_s(\vec{\kappa},\omega)\right\}$$

The scattering law $S(\vec{\kappa},\omega)$ is composed of two parts

$$S(\vec{\kappa},\omega) = S_s(\vec{\kappa},\omega) + S_d(\vec{\kappa},\omega)$$

Van Hove's space-time formulation

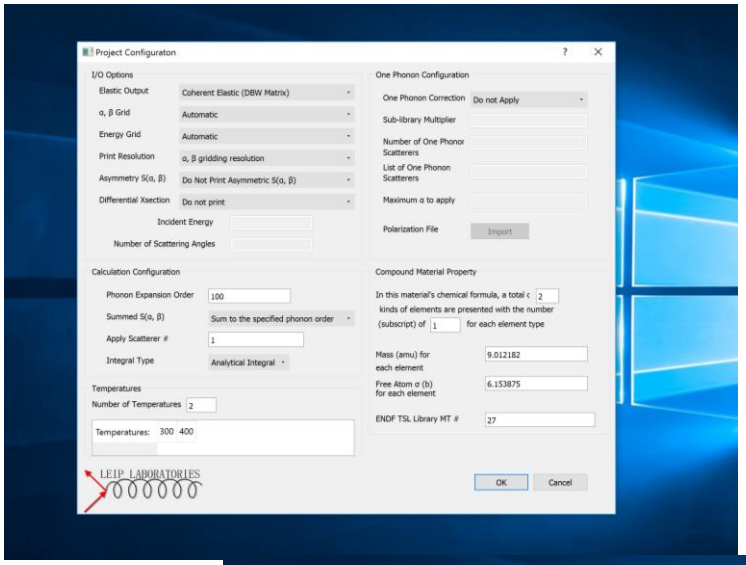
$$I(\vec{\kappa},t) = \int G(\vec{r},t)\exp(i\vec{\kappa}\cdot\vec{r})d\vec{r}$$

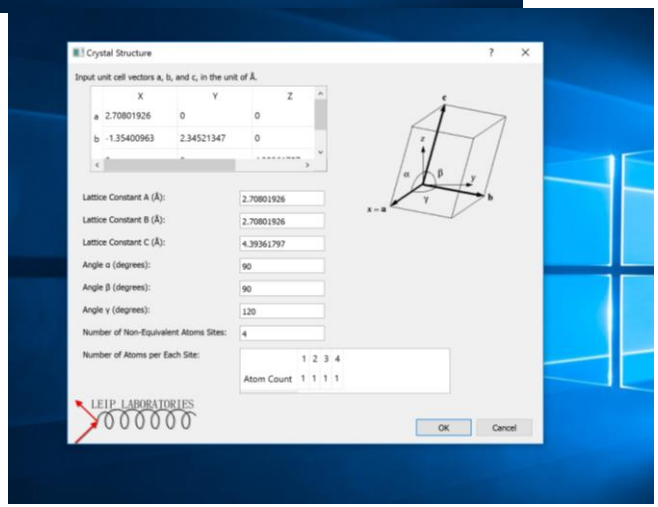
$$S(\vec{\kappa},\omega) = \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} G(\vec{r},t)e^{i(\vec{\kappa}\cdot\vec{r}-\omega t)}d\vec{r}dt$$

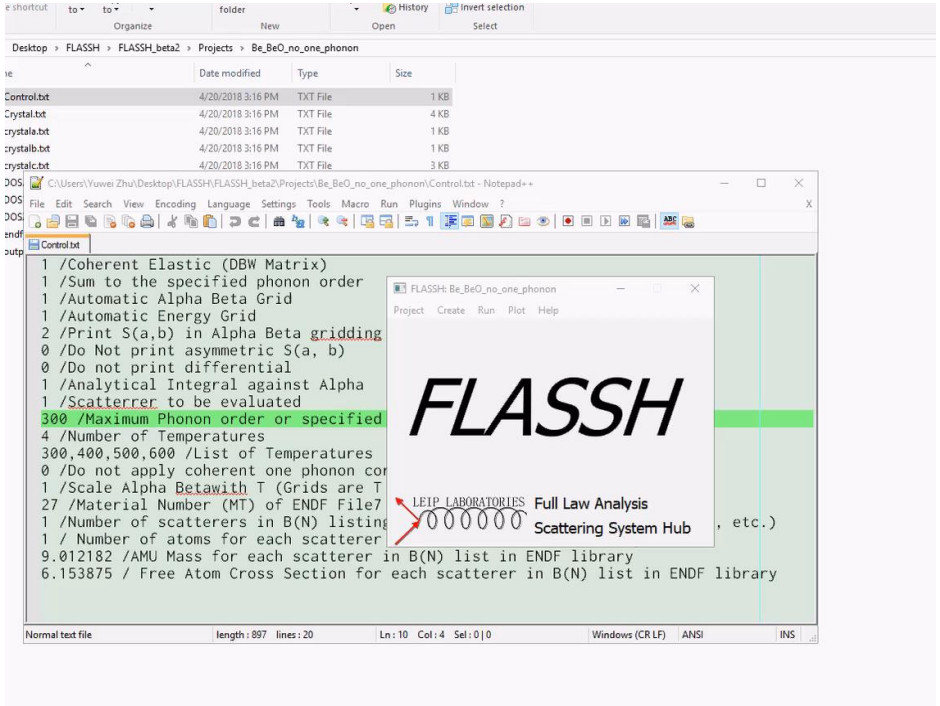
21st Century

where $G(\vec{r},t)$ is the *dynamic pair correlation function* and can be expressed in terms of time dependent atomic positions.

FLASSH Code


Project Configuraton
I/O Options
Elastic Output
Coherent Elastic (DBW Matrix)
α, β Grid
Automatic
Energy Grid
Automatic
Print Resolution
α, β gridding resolution
Asymmetry S(α, β)
Do Not Print Asymmetric S(α, β)
Differential Xsection
Do not print
Incident Energy
Number of Scattering Angles
One Phonon Configuration
One Phonon Correction
Do not Apply
Sub-library Multiplier
Number of One Phonon Scatterers
List of One Phonon Scatterers
Maximum α to apply
Polarization File
Import
Calculation Configuration
Phonon Expansion Order
100
Summed S(α, β)
Sum to the specified phonon order
Apply Scatterer #
1
Integral Type
Analytical Integral
Compound Material Property
In this material's chemical formula, a total of
2
kinds of elements are presented with the number
(subscript) of
1
for each element type
Mass (amu) for each element
9.012182
Free Atom σ (b) for each element
6.153875
ENDF TSL Library MT #
27
Temperatures
Number of Temperatures
2
Temperatures:
300 400
OK
Cancel
LEIP LABORATORIES


Crystal Structure
Input unit cell vectors a, b, and c, in the unit of Å.
X
Y
Z
a 2.70801926 0 0
b -1.35400963 2.34521347 0
Lattice Constant A (Å):
2.70801926
Lattice Constant B (Å):
2.70801926
Lattice Constant C (Å):
4.39361797
Angle α (degrees):
90
Angle β (degrees):
90
Angle γ (degrees):
120
Number of Non-Equivalent Atoms Sites:
4
Number of Atoms per Each Site:
1 2 3 4
Atom Count 1 1 1 1
OK
Cancel
LEIP LABORATORIES

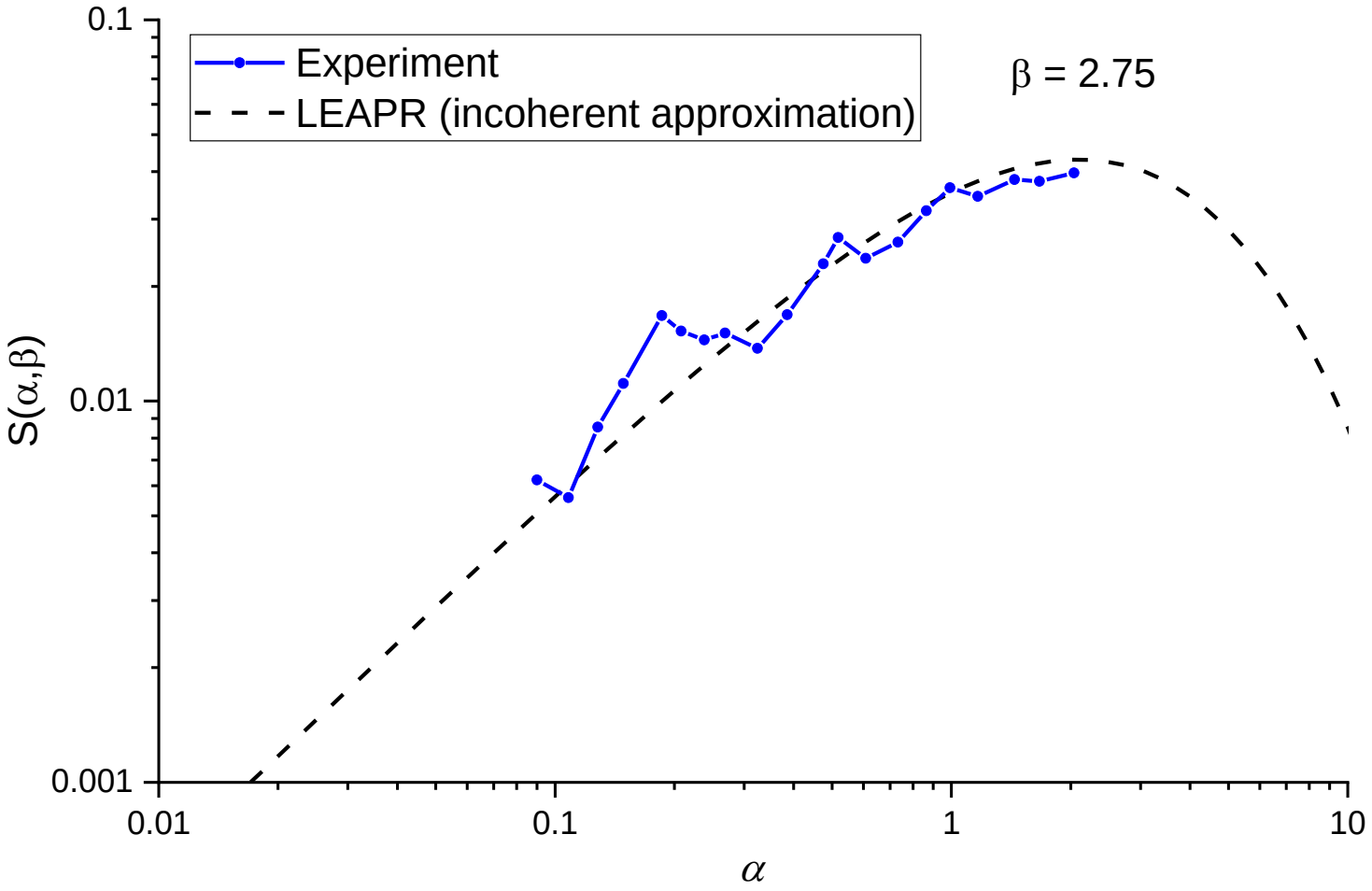

Desktop › FLASSH › FLASSH_beta2 › Projects › Be_BeO_no_one_phonon
Control.txt
Crystal.txt
crystala.txt
crystalb.txt
crystalc.txt
Date modified
Type
Size
4/20/2018 3:16 PM
TXT File
1 KB
4 KB
1 KB
1 KB
3 KB
C:\Users\Yuwei Zhu\Desktop\FLASSH\FLASSH_beta2\Projects\Be_BeO_no_one_phonon\Control.txt - Notepad++
1 /Coherent Elastic (DBW Matrix)
1 /Sum to the specified phonon order
1 /Automatic Alpha Beta Grid
1 /Automatic Energy Grid
2 /Print S(a,b) in Alpha Beta gridding
0 /Do Not print asymmetric S(a, b)
0 /Do not print differential
1 /Analytical Integral against Alpha
1 /Scatterrer to be evaluated
300 /Maximum Phonon order or specified
4 /Number of Temperatures
300,400,500,600 /List of Temperatures
0 /Do not apply coherent one phonon cor
1 /Scale Alpha Betawith T (Grids are T
27 /Material Number (MT) of ENDF File7
1 /Number of scatterers in B(N) listing
1 / Number of atoms for each scatterer
9.012182 /AMU Mass for each scatterer in B(N) list in ENDF library
6.153875 / Free Atom Cross Section for each scatterer in B(N) list in ENDF library
, etc.)
FLASSH: Be_BeO_no_one_phonon
Project Create Run Plot Help
FLASSH
LEIP LABORATORIES
Full Law Analysis
Scattering System Hub
Normal text file
length : 897 lines : 20
Ln : 10 Col : 4 Sel : 0 | 0
Windows (CR LF)
ANSI
INS

FLASSH Code Features

	NJOY (LEAPR and THERMR)	*FLASSH*
Incoherent approximation	Yes	No
Cubic approximation	Yes	No
One atom per unit cell	Yes	No
Short Collision Time (SCT) Approximation	Yes	No
Coherent elastic scattering	Approximate (and hard coded for selected materials)	Exact formulation (any material based on user input)
Integral against α	Numerical	Analytical (optional numerical)
α,β grid	User input	Automatic (optional user input)
Parallel computing	N/A	Yes
Input syntax check	N/A	Yes
Graphical user interface	N/A	Yes

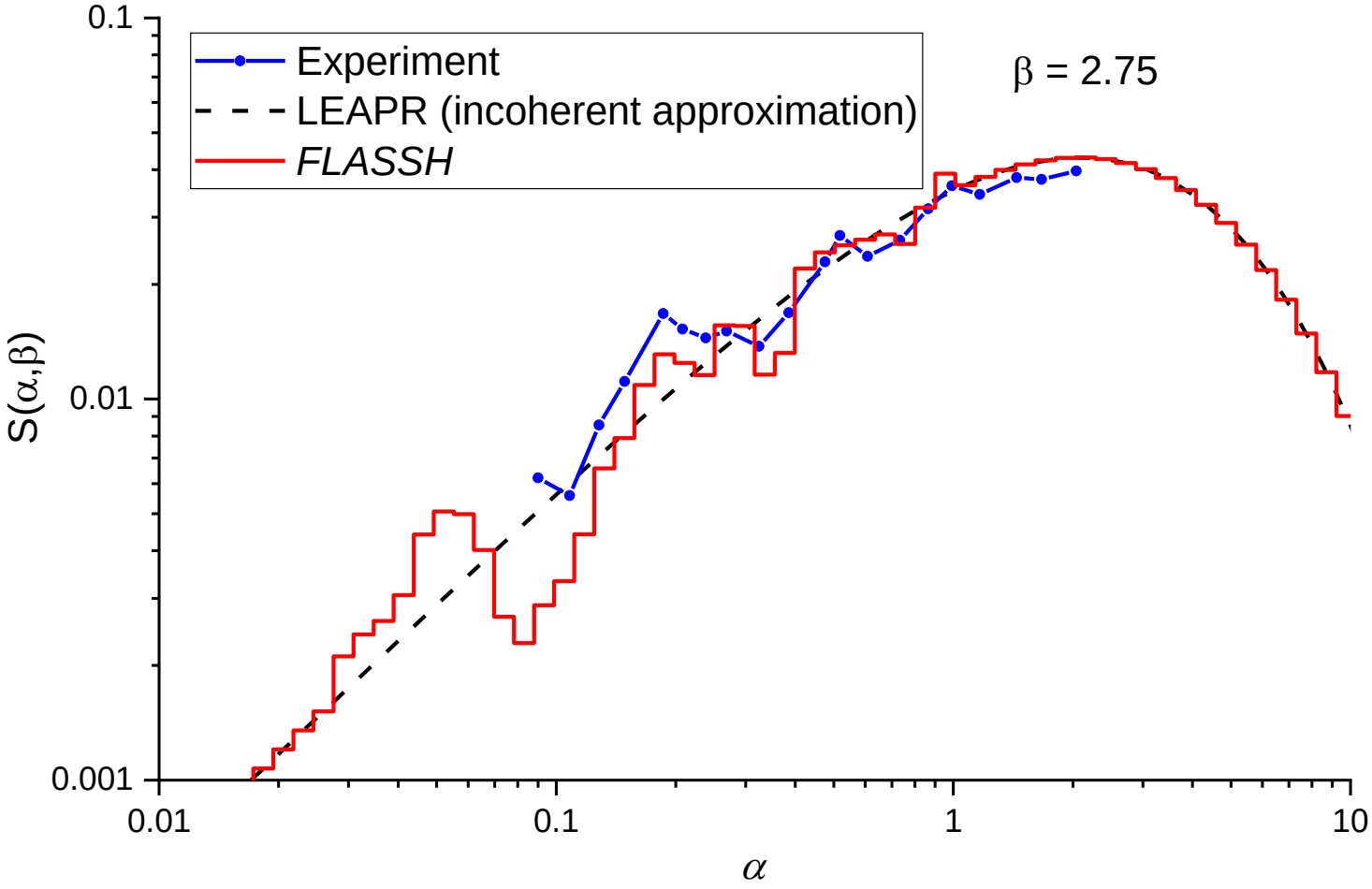
NJOY

Be Scattering Law $S(\alpha, \beta)$



FLASSH

Be Scattering Law $S(\alpha, \beta)$



Summary

- New NEUP project (Nuclear Data) to evaluate TSL for FLiBe, C-C composites, and Nuclear Graphite
- Modern predictive methods for thermal neutron cross section calculations based on the use of atomistic simulations
  - Ab initio lattice dynamics
  - Molecular dynamics (ab initio and classical)
    - New materials
    - All states of matter (solid, liquid, gas)
    - Imperfect structure
- *FLASSH* is a new thermal scattering analysis platform that uses a generalized theoretical approach for TSL calculations.
- Developed a holistic and coupled computational-experimental approach for investigating TSL development.

Acknowledgment

- DOE NE through the Nuclear Energy University Program (NEUP)
- Nuclear Criticality Safety Program (NCSP) in collaboration with LLNL
- Naval Nuclear Propulsion Program (NNPP)

Thank You

https://www.ne.ncsu.edu/nrp/