# Investigation and Evaluation of Thermal Neutron Scattering in Nuclear Graphite

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### Acknowledgement

### ☐ The LEIP Team













- ☐ Funding by the various US agencies including DOE-NE, NSF, NNSA
- □ Collaborations with colleagues at many universities, national laboratories, and industry



### **Advanced Nuclear Reactors**



### DOE-NE

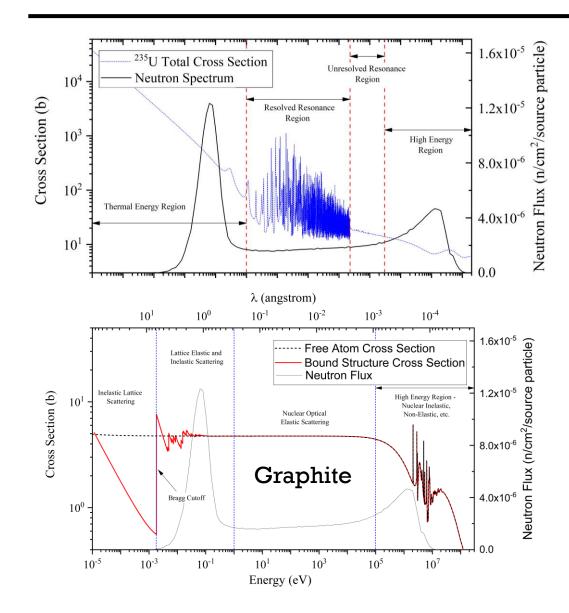


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Lead	Reactor Name	Reactor Type	Neutron Spectrum	Fuel Type	Power	Enrichment (wt% <sup>235</sup> U)	Moderator	Reflector	Coolant
TerraPower	Natrium	SFR	Fast	Sodium-bonded Metallic Alloy U-10Zr Pins	345 MWe	19.75	N/A	_	Salt
X-energy	Xe-100	Pebble Bed HTGR	Thermal	UCO TRISO Particle Spherical Graphite Compacts	80 MWe	15.5	Graphite	Graphite	Helium
Kairos Power	KP-FHR	Pebble Bed FHR	Thermal	UCO TRISO Particle Annular Spherical Graphite Compacts with Low-Density Graphite Cores	140 MWe	19.55	Pyrolytic Graphite, FLiBe	Graphite	FLiBe
Westinghouse Nuclear	eVinci	Heat-pipe Microreactor	Thermal	UCO TRISO Particle Cylindrical Graphite Compacts	5 MWe	19.75	Graphite	_	Sodium Heat Pipes
Southern Company and TerraPower	MCFR	MSR	Fast	Dissolved Uranium in Salt (NaCl-UCl <sub>3</sub> )	800 MWe	HALEU	N/A	_	Salt
BWXT	BANR	HTGR	Thermal	UN TRISO in SiC/Carbon Matrix Compact, Additively Manufactured	50 MWth	19.75 (Baseline Design)	Graphite	_	Helium
ARC	ARC-100	SFR	Fast	Sodium-bonded U-10Zr pins	100 MWe	20 Max.; 13.1 Avg.	N/A	Stainless Steel	Sodium
GA-EMS	FMR	GFR	Fast	UO <sub>2</sub> Pellets	44 MWe	19.75	N/A	Zr <sub>3</sub> Si <sub>2</sub> and Graphite	Helium
MIT	HC-HTGR	HTGR	Thermal	TRISO Particle Graphite Compact	~58 MWth	_	Graphite	_	Helium



### **Thermal Nuclear Reactor**



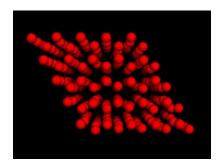
Fission

$$R_f = N \int \sigma_f(E) \phi(E) dE$$

**Thermalization** 

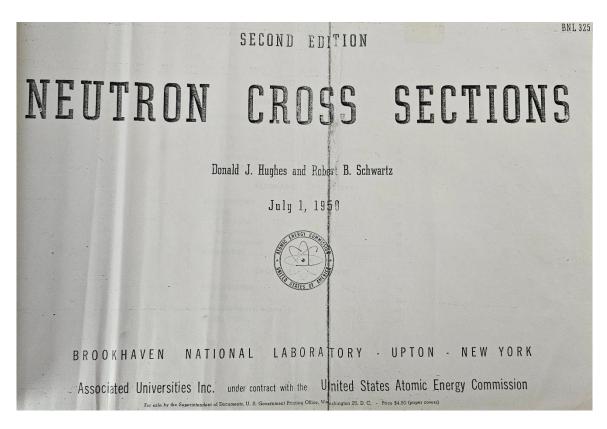
$$\frac{\partial^2 \sigma}{\partial \Omega \partial E'} = \frac{1}{4\pi} \sqrt{\frac{E'}{E}} \left[ \sigma_{coh} S(\alpha, \beta) + \sigma_{inc} S_s(\alpha, \beta) \right]$$

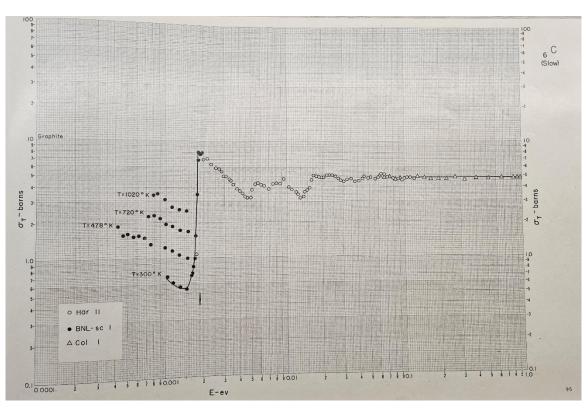
$$S(\alpha, \beta) = \frac{1}{k_{\scriptscriptstyle B} T} \frac{1}{2\pi\hbar} \int e^{i(\vec{\kappa} \cdot \vec{r} - \omega t)} G(\vec{r}, t) d\vec{r} dt$$



Moderator microstructure dictates the physics, operations, and safety of the reactor

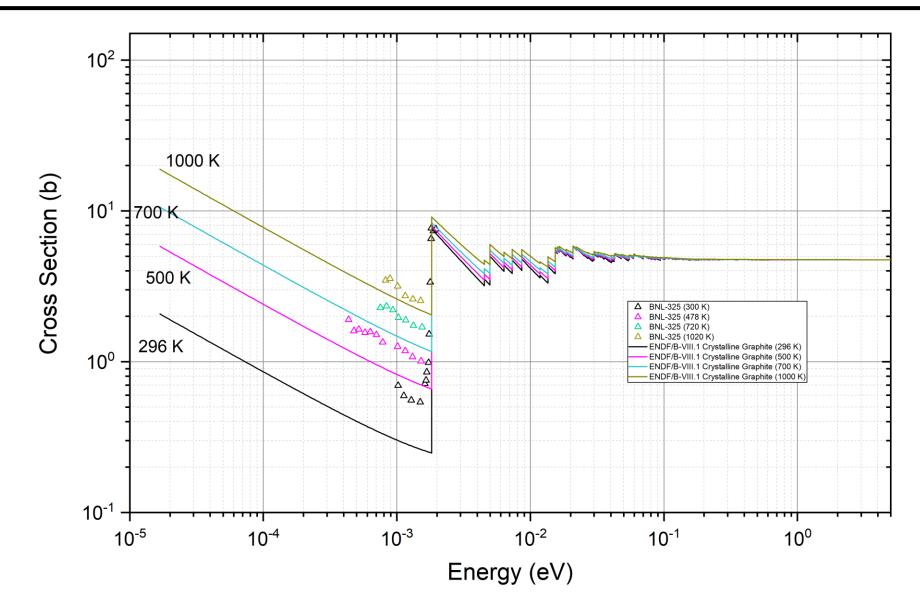
### Graphite - What's the Problem (1950s)?







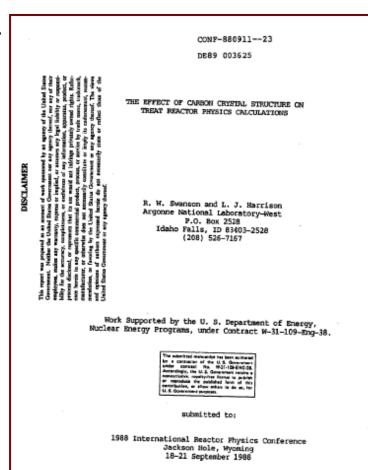
### Graphite - What's the Problem (1950s)?





### Graphite - What's the Problem (1980s)?

- Graphite reactor behavior
  - Criticality
  - Fission rates
  - ☐ Feedback
- Solution (ad hoc)
  - Assume crystalline (ideal) graphite structure (i.e., ideal  $S(\alpha, \beta)$ , but use "nuclear graphite" density (1.6-1.8 g/cm<sup>3</sup>)
  - Mix crystalline graphite and free atom libraries to improve results.



### Table II Calculated Values of k-effective

Calculational Description		cription	k-effective
Loading 1341	100%	Graphite	$0.9724 \pm 0.0021$
Loading 1341	59%	Graphite	0.9921 ± 0.0012
Loading 1343	100%	Graphite	0.9707 + 0.0024
Loading 1343	59%	Graphite	0.9922 ± 0.0017

### Table III Calculated Fission Density Ratios

Calculational Description	Calculated Fission Density Ratio	CalcExp. Exp.	
100% Graphite	43.2 ± 1.4	+6.9%	
59% Graphite	39.4 ± 1.2	-2.5%	



### Graphite - What's the Problem (2020s)?

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ARTICLE



### A pseudo-material method for graphite with arbitrary porosities in Monte Carlo criticality calculations

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### ABSTRAC

The latest ENDF/B-VIII library adapted new porosity-dependent cross-section data of graphite. However, the porosity of the actual graphite does not necessarily correspond to the porosity given in the data. We have proposed a method to perform neutronic calculations at the desired porosity on the basis of the pseudo-material method. We have also compared the  $k_{\rm def}$  values calculated by the pseudo-material method. We have also compared the  $k_{\rm def}$  values calculated by the pseudo-material method with the experimental values for the VHTRC. In addition, we have investigated the temperature dependance of the calculation values obtained by this method. From these results, we have concluded that this method allows us to perform the neutronic calculations in which we can reflect detailed information on the porosity of graphite. ARTICLE HISTORY Received 8 January 2021 Accepted 26 February 2021

### ENDF/b-viii; graphite; porosity-dependent crosssection data; vhtrc; pseudo

### material method

### 1. Introduction

In recent years, the high temperature gas-cooled reactor (HTGR) has attracted much interest as one of the Generation IV nuclear reactor systems. One of the notable features of the HTGR is that graphite is used not only as a moderator but also as a structural material owing to its excellent thermal and mechanical properties under the high temperature environment. A large amount of graphite is placed in the HTGR core so that the neutrons are sufficiently moderated. Therefore, the accuracy of neutronic calculation of the HTGR is highly dependent on the nuclear data of graphite. Especially, the thermal scattering law (TSL) data of graphite, which impacts the neutron energy spectrum, is fundamental to the detailed design and core analysis of the HTGR. In IENDL-4.0 [1], the TSL data of graphite is evaluated on the basis of the traditional evaluation model of Young and Koppel [2]. On the other hand, the latest ENDF/B-VIII.0 library adopted new TSL data of graphite [3]. It has the TSL data that depends on the porosities of graphite: crystalline graphite (i.e. graphite with a porosity of 0%), reactor graphite with a porosity of 10% and reactor graphite with a porosity of 30%. This is expected to result in more accurate neutronic calculations than

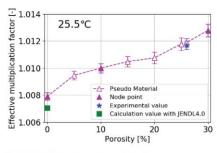
However, the actual graphite does not necessarily correspond to these porosities in the new TSL data. For instance, the density and porosity for some major graphite are shown in Table 1 [4–7], where the theoretical density of graphite is 2.25 g/cm<sup>3</sup> [8]. These values are neither 10% nor 30%. Currently, we can

only handle neutronic calculations for three porosities of 0%, 10%, and 30%. In neutronic calculations for the cores containing graphite with other than the porosities mentioned above, the nearest TSL data will be selected for use. From the viewpoint of HTGR designers, it is desirable to be able to perform neutronic calculations using graphite with any porosity. Such calculations can eliminate the uncertainties associated with the difference between the porosity of actual graphite and the porosity given in the calculation input.

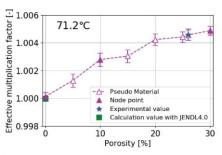
The purpose of this study is to propose a practical method for performing accurate neutronic calculations reflecting detailed information on the porosity of graphite. The proposed method allows us to perform neutronic calculations at any porosities between 0% and 30%. Using the Very High Temperature Reactor Critical Assembly (VHTRC) [9], criticality calculation results based on the proposed method are also described making comparisons with experimental results.

### 2. Methodology

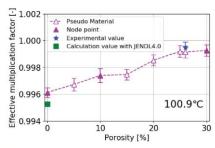
The pseudo-material method is applied to a material containing graphite to perform neutronic calculations with the specified porosity. The pseudo-material method was originally developed by Conlin et al. in order to reduce the cross-section data for the huge temperature points [10]. In this method, a pseudo-material is defined such that a material at a certain



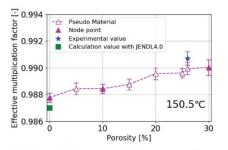
**Figure 6.** Calculation results of the  $k_{\rm eff}$  values at 25.5  $\Box$  using graphite with each porosity.



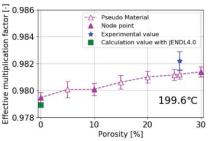
**Figure 7.** Calculation results of the  $k_{\text{eff}}$  values at 71.2  $^{\circ}$ C using graphite with each porosity



**Figure 8.** Calculation results of the  $k_{\text{eff}}$  values at 100.9  $^{\circ}\text{C}$  using graphite with each porosity.



**Figure 9.** Calculation results of the  $k_{\rm eff}$  values at 150.5  $^{\circ}{\rm C}$  using graphite with each porosity.



**Figure 10.** Calculation results of the  $k_{\rm eff}$  values at 199.6°C using graphite with each porosity.

MVP-3, JENDL4.0 Crystalline (0% porosity) Graphite TSL

Temp.	Benchmark	C/E (pcm)
25.5°C	1.0115 ± 0.0032	-444
71.2°C	1.0046 ± 0.0033	-462
100.9°C	0.9994 ± 0.0035	-413
150.5°C	0.9906 ± 0.0035	-360
199.6°C	$0.9820 \pm 0.0037$	-307

# LEIP LABORATORIES

### Thermalization – Modern History (2000-2012)

### U.S. DEPARTMENT OF ENERGY NUCLEAR ENERGY RESEARCH INITIATIVE ABSTRACT

PI: Ayman I. Hawari, Ph. D. Proposal No.: 01-140

Institution: University of Cincinnati

Title: Development and Validation of Temperature Dependent Thermal Neutron

Scattering Laws for Applications and Safety Implications in Generation IV

**Nuclear Reactor Designs** 

The University of Cincinnati (UC), Oak Ridge National Laboratory (ORNL), and the Institute Balseiro (IB) propose to perform theoretical, computational, and experimental investigations on temperature dependent neutron thermalization in moderating materials that are of major importance to the safety of nuclear systems. The objectives of this work are: to critically review the currently used thermal neutron scattering laws for various moderators and fuel cells as a function of temperature, to use the review as a guide in examining and updating the various computational approaches in establishing the scattering law, to understand the implications of the obtained results on the ability to accurately define the operating and safety characteristics (e.g. the moderator temperature coefficient) of a given reactor design -- that is, to know not only the reactivity coefficients but also their errors, sensitivity coefficients and covariance matrices, to develop and generate new sets of temperature dependent thermal neutron scattering laws,  $S(\alpha,\beta)$ , either by an evolutionary process or by changing the models entirely (e.g., introducing the coherent part of the inelastic scattering or using the synthetic kernel approach), and finally to test and benchmark the developed models within the framework of a neutron slowing down experiment. In particular, the studies will concentrate on investigating the latest ENDF/B thermal neutron cross sections for reactor grade graphite, beryllium, beryllium oxide, zirconium hydride, high purity light water, and polyethylene at temperatures greater than or equal to room temperature. These materials are neutron moderators/reflectors that will be used in the development of Generation IV nuclear power reactors and in many applications in the nuclear science and engineering field. Of major importance is graphite, which is the moderator in the modular pebble bed reactor (MPBR) that is being examined internationally as a possible Generation IV power reactor, as the subcritical reactor in accelerator driven concepts, and as the incinerator of radioactive waste and weapon's plutonium. Furthermore, a newly developed highly conductive form of graphite, known as graphite foam, is currently under study as a reactor material. Added to that, these materials of interest in research reactors such as zirconium hydride (i.e., TRIGA), and in Nerva derivative power sources for space applications (e.g., zirconium hydride, Be and BeO reflectors).

To begin this work, we will perform a critical analysis of the models that are the basis of the present ENDF/B evaluation of the scattering law for a given moderator, and determine the sensitivity of calculated thermal neutron spectra to the details and parameters of the models. Furthermore, we will consider the impact of model parameters on the behavior of the neutron flux around nearby neutron absorption resonances that are going to define global quantities such as the asymptotic neutron spectra and, consequently, reactivity coefficients. We will also study the impact of model parameters on other measured observables such as neutron pulse and wave propagation parameters, and decay constants as a function of size and transuranium buildup and depletion. In addition, we will examine the latest developments in

Continued 01-140

thermalization theory and condensed matter physics. Experiments, like the direct measurement of the double differential cross sections and specific heats, and theoretical developments (e.g., new phonon distribution in graphite) will be evaluated to define the degrees of freedom of the scattering media as well as the mechanisms for the transference of energy between the media and the neutrons. All this information will be included as input for new calculations of the scattering matrices with an updated version (to be developed as part of this research) of the present "state of the art" computer codes (used for ENDF/B compilations). As a result, thermal scattering laws,  $S(\alpha, \beta)$ , will be regenerated using basic input data and modern computational methods. Using these new sets of  $S(\alpha, \beta)$ , we will analyze the computational anomalies in the thermal scattering data that is in general use today and can cause "strange" behavior in the computational determination of the temperature coefficient of reactivity in nuclear reactors. Discrepancies of up to 150% have been encountered, which may have important safety implications [1]. Consequently, the impact of condensed matter models, and their respective input parameters, on the temperature coefficient of reactivity in nuclear reactors will be determined. Moreover, the computationally regenerated scattering data for the moderators of interest will be used in neutronics calculations of the temperature coefficients of reactivity for several Generation IV nuclear power reactors (e.g., MPBR).

Finally, since graphite is the moderator in various Generation IV reactor concepts, we will benchmark the developed  $S(\alpha,\beta)$  model for graphite by performing a neutron thermalization experiment in a graphite (and if available in graphite foam) moderator that is driven by a pulsed neutron source. This measurement approach has the ability to observe the neutron behavior in a moderator as it passes through the slowing down and thermalization energy ranges before its diffusion and escape. Therefore, it is applicable to measurements in the energy range below 1 eV, which is not accessible using the traditional out-of-pile leakage spectrum measurements. The experiment will take place using the Oak Ridge Electron Linear Accelerator (ORELA) facility, and will be performed to obtain the integral time dependent reaction rate of a neutron detector that is placed within the moderator at various temperatures greater than or equal to room temperature (including temperatures encountered in normal operations and during reactor accident conditions). In addition, a beam will be extracted from the moderator to perform temperature dependent measurements (using the ORELA time of flight facilities) of the thermal neutron energy spectrum in the moderator. We will also introduce the new graphite  $S(\alpha, \beta)$  data into time and energy dependent 3-D Monte Carlo (e.g., MCNP) computer simulations of the experiments. This will provide computational predictions of the experimental data and will enable validation of the nuclear data libraries for graphite in the thermal energy region.

### **Major outcomes**

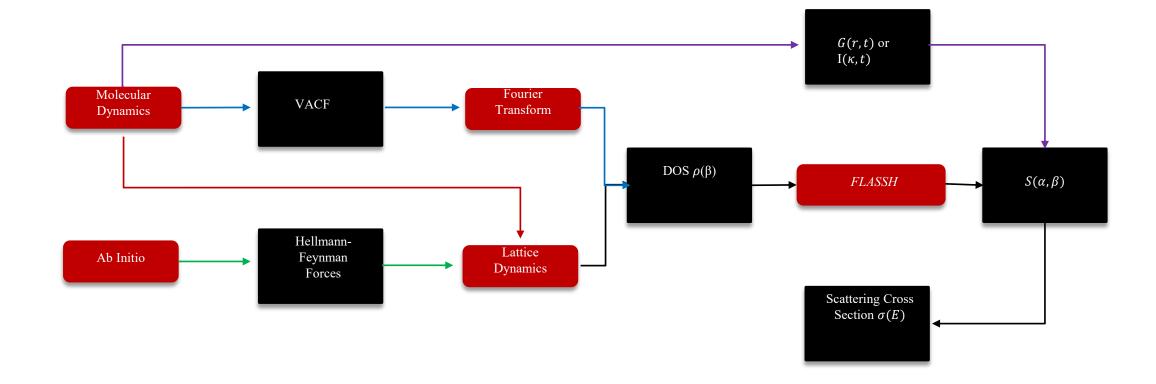
- Modern condensed matter physics methods (AILD and MD)
- 2) Modern scattering theory (removed many approximations)
- 3) Several experiments including Pulsed neutron slowing down benchmark methods

### Thermalization – Modern History (2000-2012)

### ☐ A selection of computational routes

Somewhat material dependent

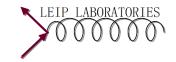


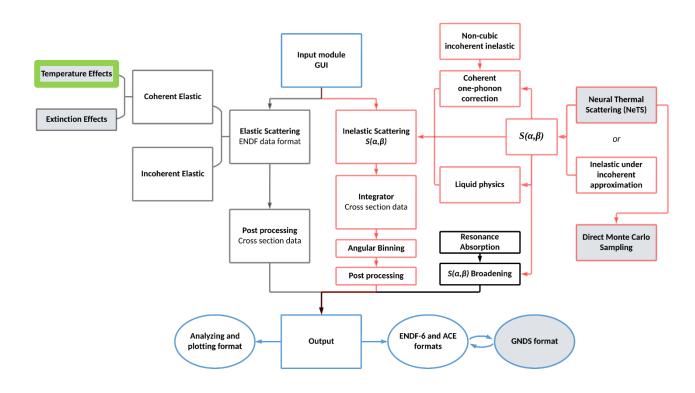


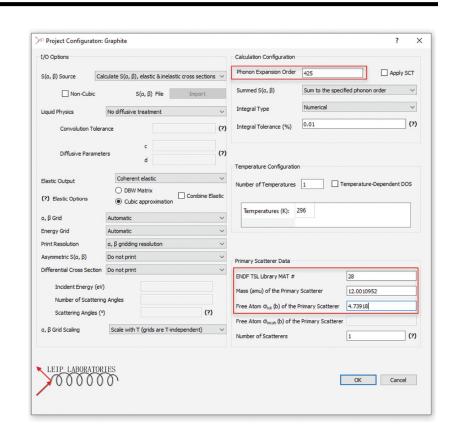




### **FLASSH**







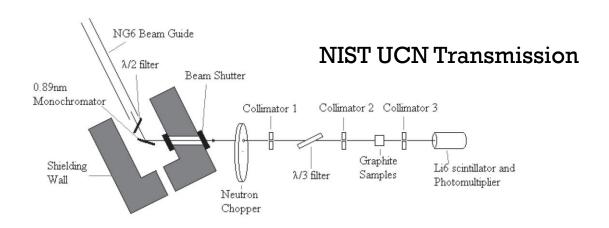
### Advanced features including

- Temperature dependent phonon spectra
- □ Coherent elastic scattering extinction effects
- NeTS modules for key moderators
- ☐ Improved liquid physics (addressing high viscosity liquids)
- Enhanced Data formatting capabilities



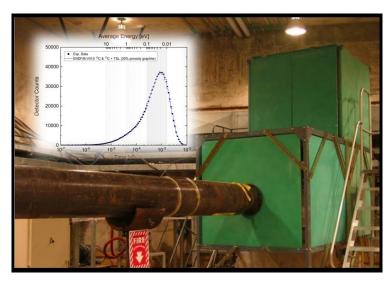
### Thermalization - Modern History (2000-2012)

### ☐ Experimental **HOLISTIC** approach

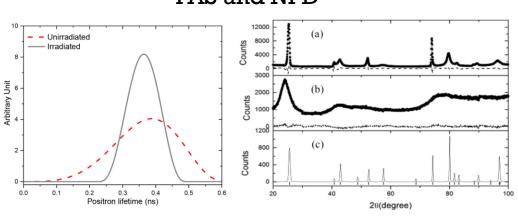


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### **ORELA Benchmark**



### PAS and NPD





### **TSL – Modern History (2000-2012)**

Available online at www.sciencedirect.com

### ScienceDirect

**Nuclear Data** Sheets

Nuclear Data Sheets 118 (2014) 172-175

### Modern Techniques for Inelastic Thermal Neutron Scattering Analysis

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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

### I. 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 hinding 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

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

http://dx.doi.org/10.1016/j.nds.2014.04.029

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

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

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

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])

$$\frac{d^{2}\sigma}{d\Omega dE} = \frac{1}{4\pi} \frac{k'}{k} \left[\sigma_{coh} + \sigma_{incoh}\right] S_{s} \left(\vec{\kappa}, \omega\right). \quad (3)$$

However, for some important neutronic materials such as graphite and beryllium, this assumption can introduce



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### ScienceDirect

Nuclear Data Sheets 118 (2014) 176-178

**Nuclear Data** Sheets

www.elsevier.com/locate/nd

### Inelastic Thermal Neutron Scattering Cross Sections for Reactor-grade Graphite

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Current calculations of the inelastic thermal neutron scattering cross sections of graphite are based on representing the material using ideal single crystal models. However, the density of reactor-grade graphite is usually in the range of 1.5 g/cm<sup>3</sup> to approximately 1.8 g/cm<sup>3</sup>, while ideal graphite is characterized by a density of nearly 2.25 g/cm<sup>3</sup>. This difference in density is manifested as a significant fraction of porosity in the structure of reactor-grade graphite. To account for the porosity effect on the cross sections, classical molecular dynamics (MD) techniques were employed to simulate graphite structures with porosity concentrations of 10% and 30%, which are taken to be representative of reactor-grade graphite. The phonon density of states for the porous systems were generated as the power spectrum of the MD velocity autocorrelation functions. The analysis revealed that for porous graphite the phonon density of states exhibit a rise in the lower frequency region that is relevant to neutron thermalization. Using the generated phonon density of states, the inelastic thermal neutron scattering cross sections were calculated using the NJOY code system. While marked discrepancies exist between measurements and calculations based on ideal graphite models, favorable agreement is found between the calculations based on the porous graphite models and measured data.

### I. INTRODUCTION

Traditionally, ENDF/B graphite evaluations provide what is known as  $S(\alpha, \beta)$  libraries to describe neutron thermalization. These evaluations are based on repre senting the material using ideal single crystal models [1] Furthermore, the libraries are generated within the inco herent approximation of thermal neutron scattering the ory. Past work showed that this approach introduced noticeable inaccuracies in the generated cross sections relative to measured data [2]. While the deficiencies due to the incoherent approximation were remedied by accounting for coherent inelastic scattering, it remained clear that the discrepancies between the measured cross sections for reactor-grade graphite and the estimates based on ideal single crystal models require a review of the atomisitic models from which these estimates were de-

Ideal graphite consists of planes (sheets) of carbon atoms arranged in a hexagonal lattice with 4 atoms per unit cell. Strong covalent bonding exits between intraplaner atoms, while the interplaner bonding (i.e., between the carbon sheets) is of the weak Van der Waals type. The planes are stacked in an "ABAB" sequence. Fig. 1 shows a representation of ideal crystalline graphite.

Alternatively, reactor-grade graphite represents a

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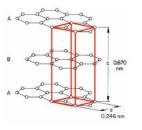


FIG. 1. The crystal structure of ideal graphite including its

multi-phase material where graphite ideal crystals are embedded in a carbon binder matrix. Most strikingly, the density of reactor-grade graphite is usually in the range of 1.5 g/cm3 to approximately 1.8 g/cm3, while ideal graphite is characterized by a density of nearly 2.25 g/cm<sup>3</sup>. This difference in density is manifested as a significant fraction of porosity in the structure of reactor-grade graphite. However, this structural feature of graphite is not captured in the process of generating the inelastic thermal neutron scattering cross sections.

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### On a measurement approach to support evaluation of thermal scattering law data



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### ARTICLE INFO

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### ABSTRACT

Inelastic thermal neutron scattering in materials that act as neutron moderators, reflectors, and filters results in shaping the neutron spectrum at low energies. This phenomenon is described using differential scattering cross sections calculated from three components including the bound atom (i.e., nuclear) scattering cross section of the neutron, the ratio of the outgoing and incoming neutron energy, and the thermal scattering law (TSL) i.e.  $S(\alpha, \beta)$  where  $\alpha$  and  $\beta$  represent dimensionless momentum and energy exchange variables, respectively. To date, no TSL libraries are generated using measured data. However, valuable information may be derived from measurements and "targeted" experiments that can validate TSL data and the related inelastic scattering cross sections. As a demonstration, a suite of coordinated measurements and experiments is described that was designed and used to support the evaluation of the TSL for "nuclear" graphite. This experimental suite includes neutron powder diffraction (for structure analysis), positron annihilation (for nano porosity assessment), inelastic neutron scattering measurements using a chopper spectrometer, transmission experiments using neutrons with energy below the Bragg cutoff thereby accessing the total (inelastic) cross section, and a slowing-down-time experiment to observe the developing neutron spectrum in the material. This experimental suite was key to understanding the difference in TSL between "nuclear" and "ideal" graphite and for the inclusion of "nuclear" graphite in the ENDF/B-VIII.0 nuclear data library release.

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### 1. Introduction

Over the past 15 years, a general methodology has been developed to generate thermal neutron scattering law (TSL) data, and calculate the inelastic thermal neutron scattering cross sections. for materials under various conditions and while relaxing many of the traditional approximations (e.g., the incoherent approximation) (Hawari, 2014, 2004). The methodology is based on using molecular dynamics (MD) and density functional theory (DFT) atomistic simulation methods to derive the fundamental input needed for TSL calculations, such as the atomic and molecular system's excitation density of states. Alternatively, the TSL may be directly accessed from the atomistic simulations and the resulting atomic correlations. In this case, corrections are needed to account for missing quantum effects such as detailed balance (Hehr. 2010). This methodology has resulted in the largest contribution (in the last 50 years) of TSL data to the recently released ENDE/B-VIII.0 nuclear data libraries (Brown, 2018).

In general, the formulation that would be the subject of the evaluation process originates from the fundamental equations for

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the double differential thermal scattering cross section. This formulation is derived using the first Born approximation of scattering theory and assumes a highly localized nuclear potential known as the Fermi pseudopotential [e.g., see Ref. Squires, 1978]. The outcome of this formulation is the following expression for the double differential thermal scattering cross section

$$\frac{d^{2}\sigma}{d\Omega dE'} = \frac{1}{4\pi k_{B}T} \sqrt{\frac{E'}{E}} [\sigma_{coh}S(\alpha, \beta) + \sigma_{inc}S_{s}(\alpha, \beta)] \qquad ($$

$$S_s(\alpha, \beta) = S_s(\alpha, \beta) + S_d(\alpha, \beta),$$
 (2)

where,  $S(\alpha, \beta)$  is the thermal scattering law,  $S_{\alpha}(\alpha, \beta)$  is the self scattering law,  $S_{\alpha}(\alpha, B)$  is the distinct scattering law,  $\alpha$  and  $\beta$  are dimensionless momentum and energy exchange variables,  $\sigma_{coh}$  is the coherent bound atom cross section,  $\sigma_{inc}$  is the incoherent bound atom cross section, E in the incoming neutron energy,  $\hat{E}$  is the scattered neutron energy,  $\Omega$  is the scattering solid angel,  $k_B$  is Boltzmann's constant, and T is the temperature of the scattering medium. In this case, S<sub>s</sub> is related to the Fourier transform in space and time of the density correlation function for an atom at a given initial location in the atomic system with its location at time t. Sd is related to the Fourier transform in space and time of the density

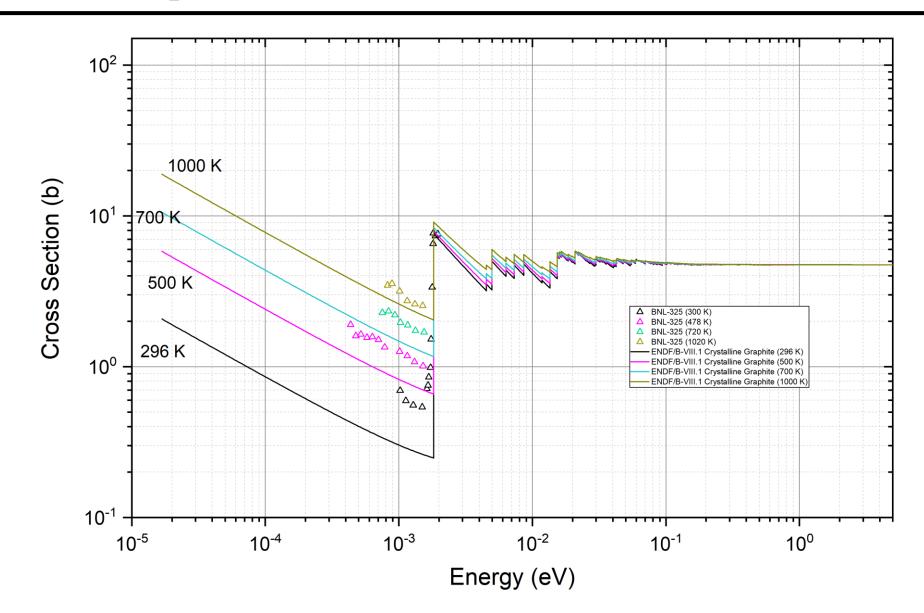


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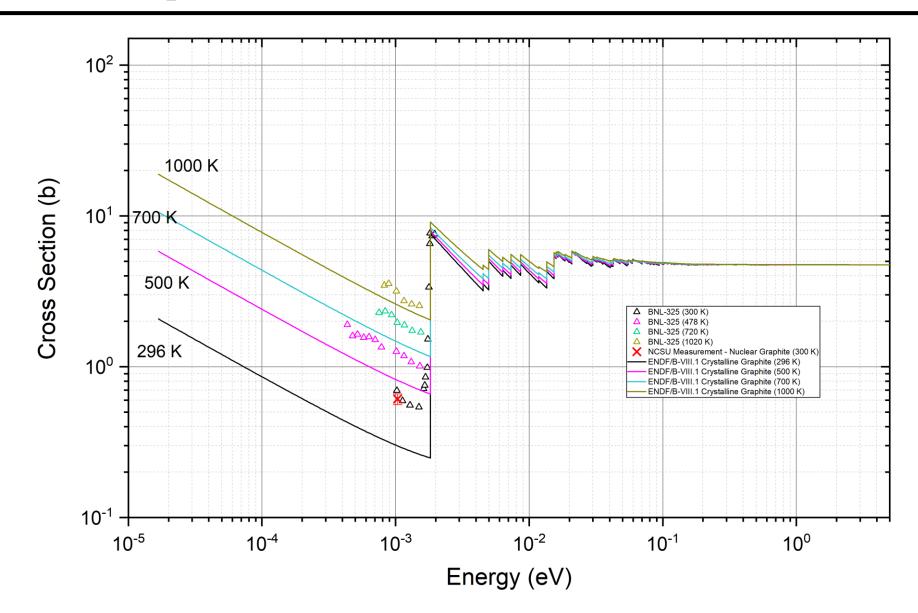
<sup>\*</sup> Corresponding author: ayman.hawari@ncsu.edu

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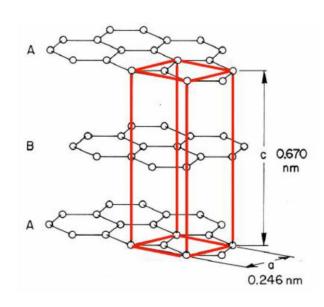
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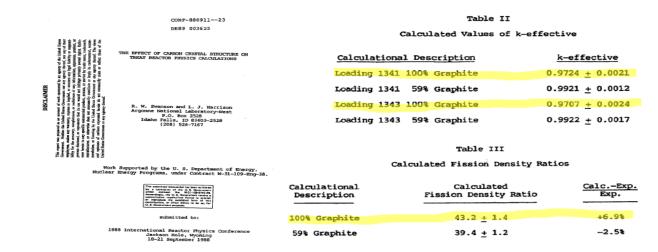


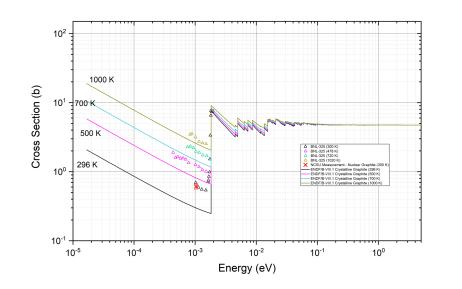






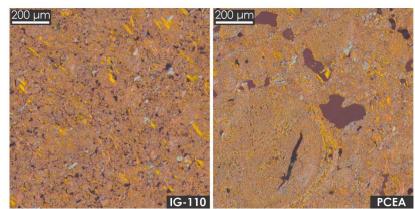
■ Model used since the 1960s and until ENDF/B-VII.1 (released in 2011).

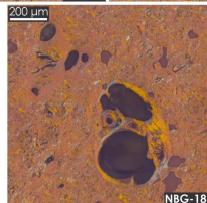


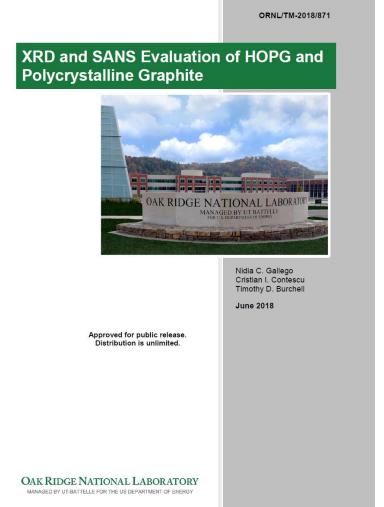


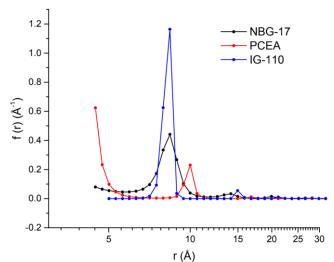


### What is Nuclear Graphite?









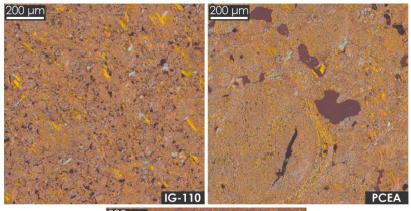


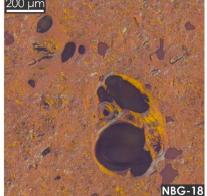


☐ Assume a nuclear graphite bulk (or pile)



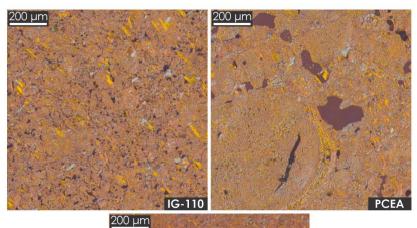
☐ Assume a nuclear graphite bulk (or pile)

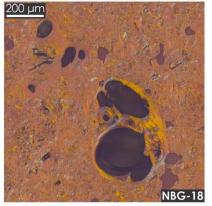


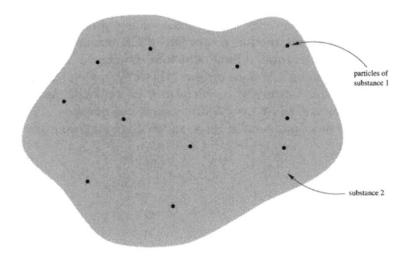




☐ Assume a nuclear graphite bulk (or pile)







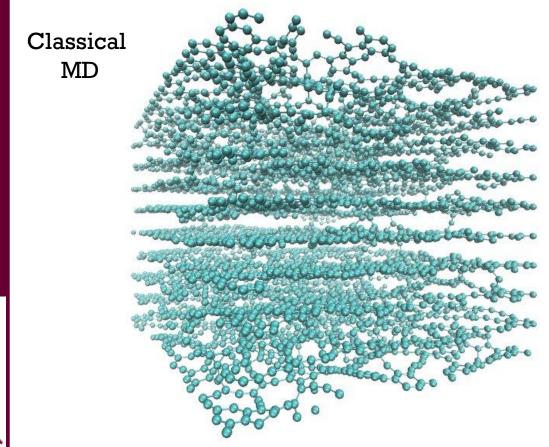
### neutronic scale

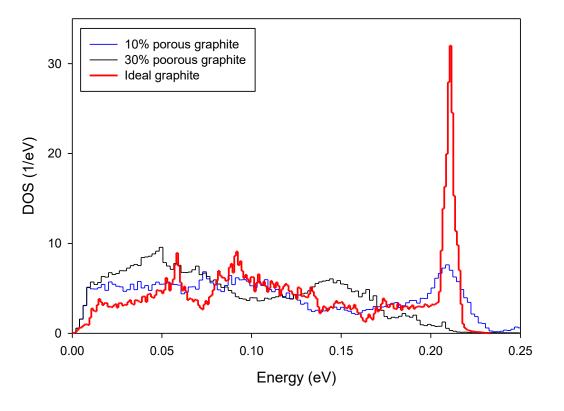
$$\mathbf{mfp} = \frac{1}{\Sigma} \approx 2.5 \text{ cm}$$



### Thermalization - Modern History (2000-2012)

- **Porous** homogeneous and uniform model of nuclear graphite model
- Conserve scattering reaction rate





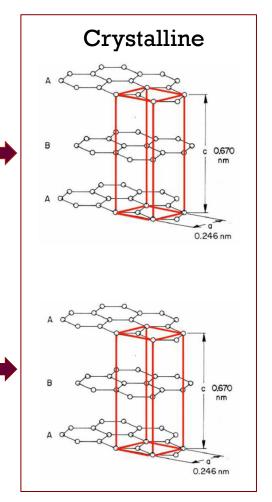
Porosity(%) = 
$$\left(1 - \frac{\rho_{nuclear\ graphite}}{\rho_{crystalline\ graphite}}\right) \times 100\%$$

### **Graphite in ENDF/B-VIII.1**

■ ENDF/B-VIII.0 and ENDF/B-VIII.1 evaluations produced for different types of graphite crystalline and nuclear (i.e., porous)

■ MT=2 block holds the coherent elastic scattering component

 $\square$  MT=4 S( $\alpha$ , $\beta$ ) block accounts for either ideal crystalline or porous (nuclear) graphite through the use of the appropriate graphite phonon DOS



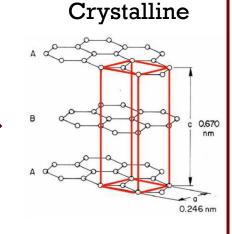


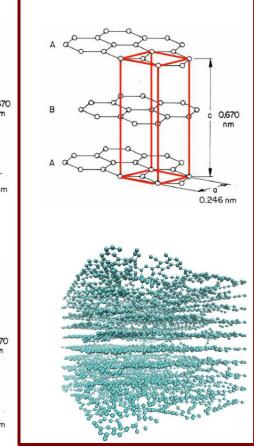
### **Graphite in ENDF/B-VIII.1**

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■ MT=2 block holds the coherent elastic scattering component

**MT=4**  $S(\alpha,\beta)$  block accounts for either ideal crystalline or porous (nuclear) graphite through the use of the appropriate graphite phonon DOS





**Nuclear** 



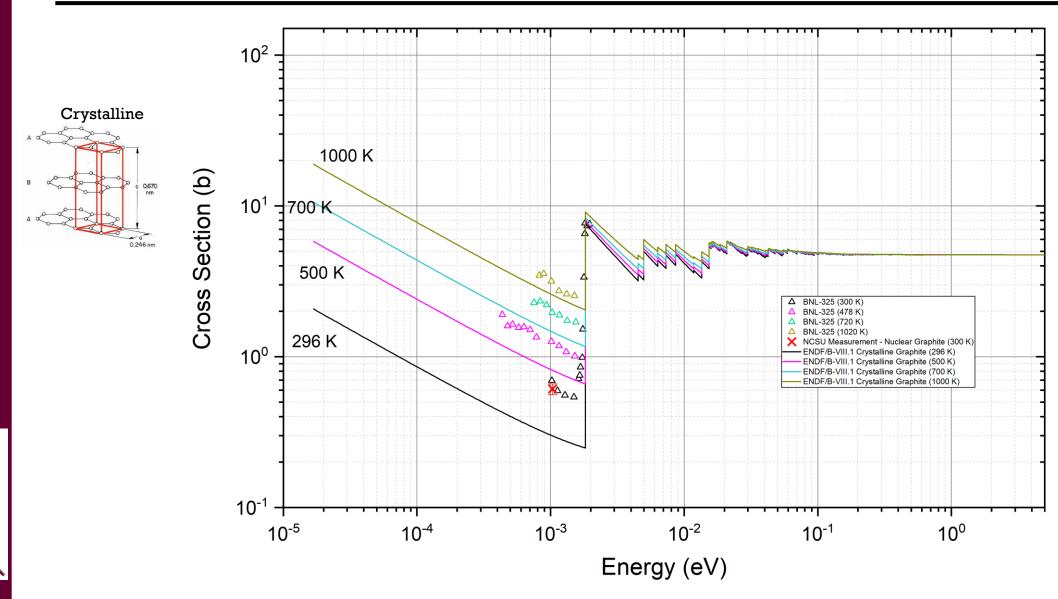
### **Graphite in ENDF/B-VIII.1**

- Five (5) variations of graphite in ENDF/B-VIII.1
  - (all evaluated by LEIP group)
  - 1. Crystalline graphite (incoherent approximation, <u>0% porosity</u>)
  - 2. Crystalline graphite (+Sd correction, <u>0% porosity</u>)
  - 3. Nuclear graphite (incoherent approximation, 10% porosity)
  - 4. Nuclear graphite (incoherent approximation, 20% porosity)
  - 5. Nuclear graphite (incoherent approximation, 30% porosity)

	Density (g/cm^3)	Library
Porosity (%) = $\begin{pmatrix} 1 & \rho_{nuclear\ graphite} \end{pmatrix} \times 100\%$	2.26	0% porous
Porosity(%) = $\left(1 - \frac{\rho_{nuclear\ graphite}}{\rho_{crystalline\ graphite}}\right) \times 100\%$	1.9-2.0	10% porous
\ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \	1.7-1.9	20% porous
	< 1.7	30% porous

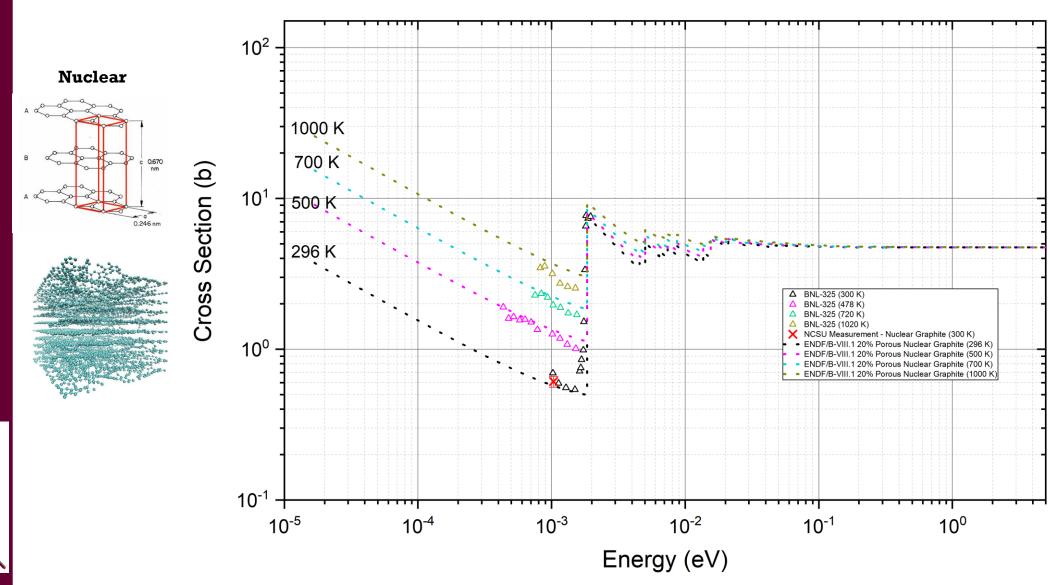
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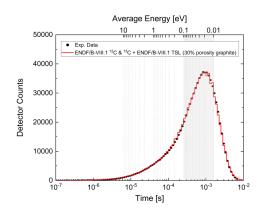


### **Nuclear Graphite – Much Improved!**





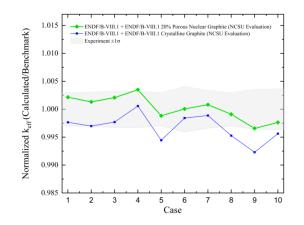
### **Nuclear Graphite - Much Improved!**



FUND-ORELA-ACC-GRAPH-PNSDT-001 (Nuclear Graphite)

Density =  $1.66 \text{ g/cm}^3$ Porosity  $\approx 30\%$ 

	Mean Absolute
<b>Cross Sections</b>	Deviation (%)
ENDF/B-VIII.0 + Cry	4.14%
ENDF/B-VIII.1 + Cry	4.09%
ENDF/B-VIII.1 + Cry +S <sub>d</sub>	5.01%
ENDF/B-VIII.1+30%	1.79%

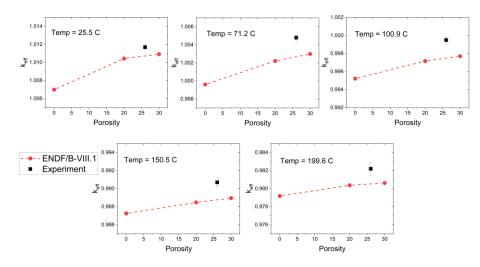


PROTEUS-GCR-EXP-001 to -004 (Nuclear Graphite)

Density = 1.7 g/cm<sup>3</sup> Porosity  $\approx$  20-30%



Case	ENDF/B-VIII.1 Crystalline	
1	235	204
2	303	137
3	230	188
4	57	322
5	707	146
6	258	12
7	83	91
8	344	95
9	782	385
10	529	247
mean	350	183
$\chi^2$	20	5



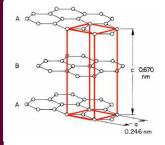
VHTRC-GCR-EXP-001 (Nuclear Graphite)

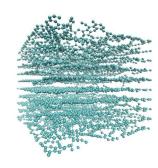
Density = 1.67 g/cm<sup>3</sup> Porosity  $\approx 30\%$ 

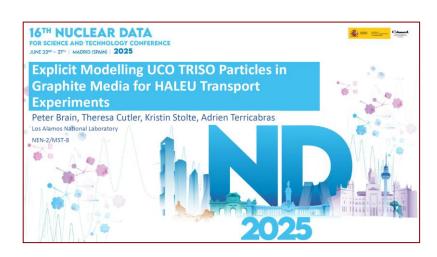
ENDF/ B-VIII.1		C-E (pcm)	
Temp.	0% Porous Crystalline Graphite	20% Porous Graphite	30% Porous Graphite
25.5°C	-462	-124	-76
71.2°C	-517	-257	-180
100.9°C	-430	-235	-181
150.5°C	-353	-228	-179
199.6°C	-314	-190	-164

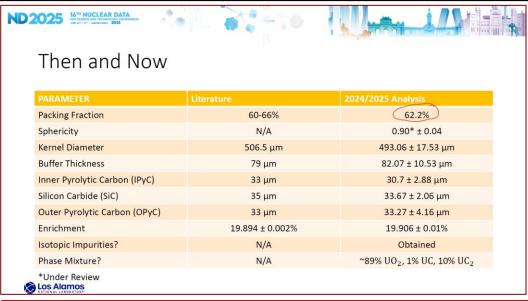
### **Nuclear Graphite – Current Testing**

### Nuclear



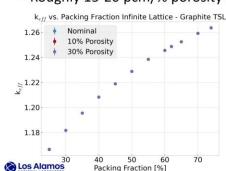


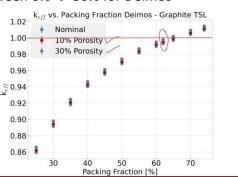




### TSL for Graphite Porosity

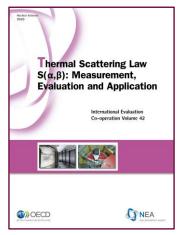
- No observable impact of TSL porosity on Infinite Lattice
  - Combination of intermediate spectra and lack of large graphite sections
- Roughly 15-20 pcm/% porosity between 0% → 30% for Deimos







### **Outcome**















ENDF/B-VIII.1: Updated Nuclear Reaction Data Library for Science and

G.P.A. Nober, <sup>1</sup>· R. Capote, <sup>2</sup> M.T. Pigni, <sup>2</sup> A. Triow, <sup>4</sup> C.M. Mattoon, <sup>5</sup> D. Neudesker, <sup>6</sup> D.A. Brown, <sup>3</sup> M.E. Chadrické, <sup>5</sup> A.C. Kahier, <sup>8</sup> N. K. Kedite, <sup>8</sup> M. Zerkie, <sup>5</sup> A. H. Swari, <sup>5</sup> C.W. Chapman, <sup>5</sup> N.C. Ferming, <sup>3</sup> J.L. Wormald, <sup>7</sup> K. Ramie, <sup>5</sup> Y. Daton, <sup>8</sup> N.A. Gibson, <sup>8</sup> P. Brain, <sup>8</sup> M.P. Paris, <sup>6</sup> G.M. Hale, <sup>6</sup> L.J. Thompson, <sup>5</sup> D. Barry, <sup>8</sup> J. Stotes, <sup>8</sup> W. Hacek, <sup>5</sup> A.E. Lowell, <sup>8</sup> M.R. Mumporee, <sup>6</sup> C. Dotel, <sup>8</sup> K. Krawaris, <sup>5</sup> C. Noguere, <sup>1</sup> J.D. McDomell, <sup>3</sup> A.D. Carlson, <sup>13</sup> M. Dumn, <sup>3</sup> T. Kawano, <sup>6</sup> D. Wardari, <sup>5</sup> L. A. Capote, <sup>5</sup> C. Soguere, <sup>1</sup> J. J. A. Carlson, <sup>5</sup> R. Capote, <sup>5</sup> C. A. Capote, <sup>5</sup> M. Carlson, <sup>5</sup> M. P. Carlson, <sup>5</sup> H. Carlson, <sup>5</sup> R. Capote, <sup>5</sup> M. Carlson, <sup>5</sup> M. Cornock, <sup>5</sup> J. Cachen, <sup>5</sup> J. P.W. Crowier, <sup>5</sup> D. E. Cullen, <sup>5</sup> A. D. Jakabakis, <sup>5</sup> M.A. Descalle, <sup>5</sup> D. D. Daldo, <sup>5</sup> P. Dimitron, <sup>5</sup> C. Cachen, <sup>5</sup> J. P. W. Crowier, <sup>5</sup> D. E. Cullen, <sup>5</sup> A. A. Jacote, <sup>5</sup> M. J. A. Bartin, <sup>5</sup> M. J. K. L. Guber, <sup>5</sup> J. D. Hartin, <sup>5</sup> M. S. K. L. Guber, <sup>5</sup> J. Darin, <sup>5</sup> M. S. Ferrer, <sup>7</sup> T. Galler, <sup>7</sup> V. Gibtert, <sup>5</sup> M. J. A. Sanghars, <sup>8</sup> M. J. Fedy, <sup>8</sup> H. K. Irach, <sup>5</sup> K. S. Kim, <sup>5</sup> A. K. Sening, <sup>5</sup> M. Kozifa, <sup>7</sup> B. K. Lamero, <sup>5</sup> A. Lamero-Case, <sup>8</sup> A. Jacote, <sup>5</sup> M. J. A. Sanghars, <sup>8</sup> M. J. K. L. Guber, <sup>5</sup> J. K. B. Carnow, <sup>5</sup> A. L. Bartin, <sup>5</sup> M. J. A. Sanghars, <sup>8</sup> M. J. K. L. Guber, <sup>5</sup> J. K. Bartin, <sup>6</sup> M. J. K. J.

Yan der Marck, M. Varnhald, <sup>15</sup> C. Wemple, <sup>25</sup> K.A. Wendt, <sup>26</sup> M. White, <sup>8</sup> and R.Q. Weight, <sup>15</sup> Pheroblaven Mittand Laboritory, Physion, NY, 11975-360; R.S. Marchardton Atomic Energy Agency, Virnin A-L(10), P.D Bur 108, Austria Challe Schmidt Endorster, Dok Roby, 77 NST3-4717, USA
 <sup>1</sup> Lawrine Liverium Valional Laboratory, Liverium C. V. S. Marchardton Atomic Laboratory, Liverium C. A. Marchardton, M. Stall, S. L. Marchardton, M. Stall, S. M. Sand, Marchardton, M. Stall, M. Marchardton, M. Stall, S. M. Sand, Marchardton, West Millin, Pennsylvania 1242-0793, USA
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 <sup>10</sup> Normal Nuclear Laboratory, Schmidten Laboratory, NY, 12430, USA
 <sup>12</sup> Challen, D. M. S. M. Schmidten, M. S. Marchardton, NY, 12430, USA
 <sup>13</sup> Spectra Tech, Inc., Ook Rolge, T. N. 3780, USA
 <sup>14</sup> Department of Nuclear, University of Shergia, Marcha, Corresony
 <sup>15</sup> Pheromatory of Nuclear Characteristics, Natural Laboratory, Schmidten Labora

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McKepfe Allermaston, Rouding, BERKSHIRES, ROT 1978.
Part Service Andrews. Annual Service Apolitics Societies (Part 1978). Service McGeller, 1978, Service McGeller, 1978, March 2078, March

<sup>31</sup> University of Serrey, Guddford, Surrey, GUZ 72H, UK (Dated: November 19, 2024; Received xx Month 2024; voice received xx Month 2024; accepted xx Month 2024). The ENDF/B-VIII. library is the newest recommended evaluated nuclear data file by the Cross

66 TSL evaluations were accepted for ENDF/B-VIII.1 for the following materials

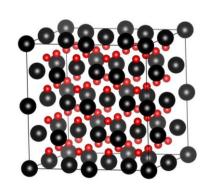
Al2O3, Be-metal, Be-metal+Sd, BeO, FLiBe, CaH2, CH2, SiC, UC, HF, Heavy Paraffinic Oil, UN, PuO2, SiO2, UO2, U-metal, Grph-10, Grph-20P, Grph-30p, Grph-cryst, Grph+Sd, Enrichment dependent fuel libraries

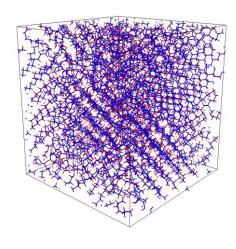
☐ FY 25 : Paraffin, U3Si2, UMo, light Paraffinic oil

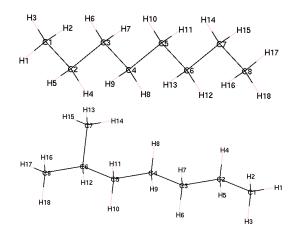


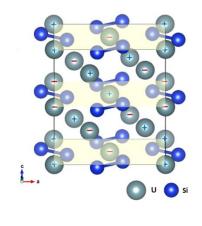
### TSLs & Beyond

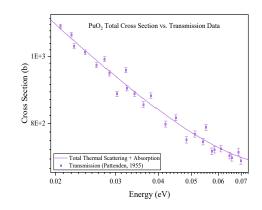
### **Thermalization – Modern History (2012-Present)**

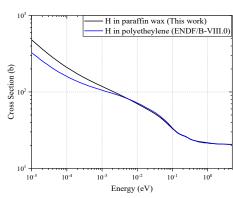


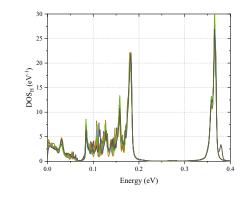


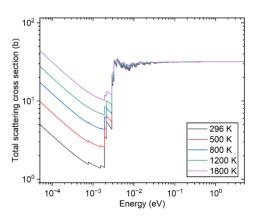












Plutonium dioxide

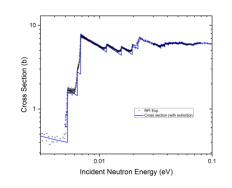
Paraffin

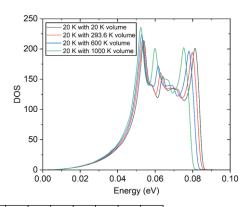
Paraffinic oil

**Uranium Silicide** 

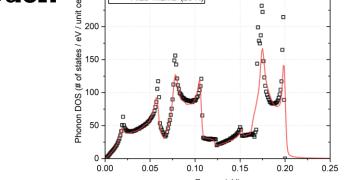
### **TSL State-of-the-Art**

- Everything developed for graphite applies to all other materials
  - ☐ Atomistic simulation methods (AILD and MD)
    - Continue to evolve
    - □ Enabled ML
  - Advanced TSL evaluation methods
    - □ FLASSH





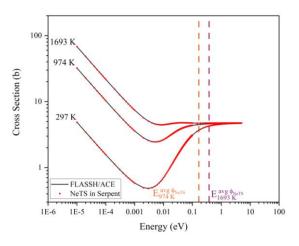
- ☐ Holistic experimental/measurement approach
  - don't pick and choose!

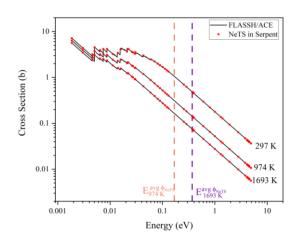


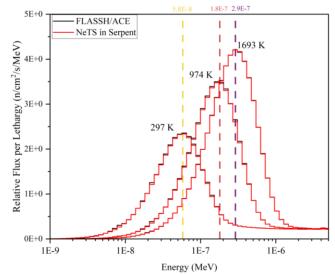
AILD (ENDF)

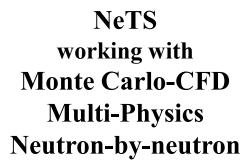


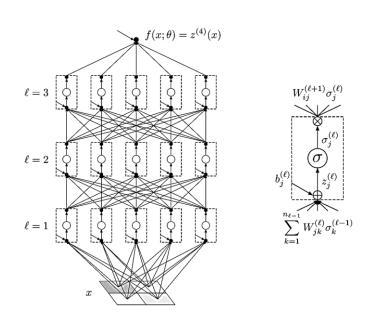
### **Thermalization – The Future**











Framework	Data Storage
ACE	~ 30 MB / Temperature
NeTS	$\sim$ 340 KB for 200+ Temperatures



### **Thermalization – The Future**

### Evaluation of Thermal Scattering Law for UsSis Using Temperature-Dependent Phonon Density of States

Junhyanna Gil. Ayman I. Hawari'

North Carolina State University, Raleigh, NC

### ABSTRACT

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Keywords: Thermal scottering law, Uranium silicide, Phonon density of states, Quasi-harmonic

### 1. INTRODUCTION

n stlicide (U<sub>3</sub>Si<sub>2</sub>) has emerged as a material for high-density and energy-efficient nuclear fuel [1] [2], [3], anticipated for application in commercial light water reactors. U<sub>1</sub>Si<sub>2</sub> has several advantages compared to maniaum dioxide (UO<sub>2</sub>), the current standard for commercial nuclear fiel. It has higher maniaum fensity than UO<sub>2</sub>, allowing a longer operating cycle and improving the efficiency of the nuclear power plant [1], [3], [4]. It also has a higher melting point and higher thermal conductivity, mitigating the risks of overheating and fuel melting and enhancing the safety of the reactor system [1], [2], [4], [5]. In addition, it potentially exhibits better resistance to radiation damage [4], which should be crucial in maintaining the integrity of both the forel and the first loads. Because of these characteristics, particularly concerning reactor safety, U,Si; has been extensively studied as a part of the accident-tolerant fuel designs [2], [4], [6] and is expected to ultimately enhance the safety and efficiency of nuclear reactor systems.

expected to transvery enables are stretch and transvery for the second polysical and thermodynamic properties of U.Sis have been addressed in experimental studies. The U.Sis crystal was found to have a tetragonal unit cell with the space group Pd-in-bar, confirmed by room temperature X-ray diffraction and high temperature neutron diffraction experiments [T], [S], [P]. Pressure dependence of the crystal structure was characterized

### crature affects on Thormal Neutron Scattering in Revellium Metal

P. G. Simeonov, J. Gil, N. C. Fleming, A. I. Hawari

pectra.

Building on prior work, this study explores the effect of



BIRMAN MAY LEAD value of the male neutrons in materials in the searching of the found neutrons in materials in the sensor same pletton 10 V is dominated by the simulation storecast and time same braiding offices. In systallant works, described and the same that the pletton of the sensor in the probability of energy and momentum transfer and the probability of energy and momentum transfer.

### Techniques for Neural Thermal Scattering (NeTS) Implementation in Neutronics Analysis

J. P. W. Crozier<sup>1</sup>, A. I. Hawari<sup>2</sup>

nt of Nuclear Engineering, North Carolina State University, Raleigh, NC 27695, USA unit of Nuclear Engineering, Texas A&M University, College Station, TX 77843, USA iperozieślinesu edą , aikawansitamu eda

The male assemble we obtained assemble the properties of the second sec

measurement extensive numeratures. A more supportant part of  $W_{ij}$  and  $W_{ij}$  respectively and  $W_{ij}$  respectively. The Thermod Savining Low CHS,  $w_i$   $S_i(\theta, \beta)$  paccounts for dynamical busining effects, and can be used to quantify the demail autience scaring practice in their cross sections). Typically, a moderated v 15th, data is evaluated in a code  $W_{ij}$  and  $W_$ 

and enhancing the fidelity of thermal scattering cross sections is to train artificial neural networks (ANNs) as universal function approximators for  $S(\alpha, \beta, T)$  [4.5.6]. These Neural Thermal Scattering (NeTS) modules collapse the complexity

n s solid moderator, the thermal neutron scottering rates
1. finetism of crystall-graphic structure and the
within of quantized lattice oscillations planeous; the
differential scottere cross services to the control of the control o

 $\frac{d^3\sigma}{d\mu dt'} = \frac{1}{2k_BT} \sqrt{\frac{\delta'}{k}} \left( \sigma_{coh} S(\alpha, \beta) + \sigma_{incoh} S_g(\alpha, \beta) \right) (1)$ 

Where S is typically evaluated in FLASSH with a observe

### $\alpha = \frac{E + \delta' - 2\mu \sqrt{EEV}}{A \log T} \ , \ \beta = \frac{E' - E}{k \pi T}$

berrowed from biology, which are mapted by the phenomenon of cognition. In the universal approximation theorem, a single-layer ANN of infinite width can approximate any continuous function [8]. In this form, the weights and biases (W<sup>0</sup><sub>1</sub>, and big<sup>1,2</sup> reportively) can be trained to interpret and learn a TSL dataset, then make

- 3. Load datasets as touch tensors into the deep learning framework, which contains a back-propagation algorithms, a neural network architecture, and
- 5. Serialize the ANN for accelerated GPU inference
- 6. Implement NeTS functionality for on-the-fly

contained within a cowlo environment has been linked with the Serpent [11] makefile, enabling NeTS TSL data

### 16TH NUCLEAR DATA

FOR SCIENCE AND TECHNOLOGY CONFERENCE

JUNE 22ND - 27TH | MADRID (SPAIN) | 2025

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Machine Learning Molecular Dynamics for Thermal Scattering Law Evaluations with Enhanced Temperature Fidelity

Junhyoung Gil and Ayman I. Hawari

North Carolina State University, Department of Nuclear Engineering, 2500 Stinson Dr. Raleigh NC 27607, USA

The thermal scattering law (TSL) quantifies the modes of energy and aumonitum transfer of low-neergy neutrons or final materials. Account TSL data are thin securitied for preferring a unifor reactor's operational and safety control of the security operational and safety control of the security operational and safety control of the security operational properties of the security operational properties of the security operational properties of the security operation operation of the security operation operation of the security operation operation

mulations are used to derive the phonon DOs for evaluating a TSL with significant accuracy. AIMD simulations asy be used to enhance fidelity and generate the DOS at finite temperatures, however, they are computationally tentientive of seeking statistically accurate DOS results. Moderated synamics (ADD using (semi-)empirical classical teratomic potentials (CP) is less computationally demanding, allowing for statistically reasonable temperature-[Lattice dynamics (AILD)]

pendent phonon DOS calculations, though the accuracy is largely affected by the parameterization of the CP.
this study, we investigate calculating the temperature-dependent phonon DOS using MD with near quantum lecular dynamics (AIMD)] anical accuracy. We proceeded by replacing the CP with a machine-learning potential (MLP) built from ab

· High computational cost; not suitable for phonon

Accuracy strongly depends on potential model

Machine-learning molecular dynamics (MLMD) Calculation of temperature-dependent phonon DOS of neutron moderator materials with near quantum mechanical accuracy by applying a machine-learning potential.

e All D/AIMD data with configurations sampled via MI MD at 20 K

SNAP was trained using ALLD AIMD data, with configurations sampled via MLMD at 20 K.
 MLMD was performed at 20 K using the trained SNAP to calculate VACF and the corresponding phonon E
 This jibnoon DOS was compared with the phonon DOS obtained via AILD to validate the overall method.
 A reasonable agreement was observed in the phonon DOS.

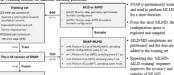
o simulation data. Machine-learning molecular dynamics (MLMD) was subsequently performed using the

sed MLP. To validate the accuracy of the fluid MLP, we calculated the phonon DOS from low-temperature MD simulations and composed is with the DOS obtained from ALID unitablions, observing good agreement, initionally, comparison of the thermal neutrino scattering cross sections calculated from the generated DOS ober derisonable consistency Subsequently, MLD immittations were conducted as executed integratures to suitable the temperature-dependent DOS, where shifts in peak positions and peak broadening with temperature observed Faility, for SLL and scattering cross sections were calculated unit get temperature-dependent observed Faility, for SLL and scattering cross sections were calculated unit get temperature-dependent observed Faility, for SLL and scattering cross sections were calculated unit get temperature-dependent observed Faility, for SLL and scattering cross sections were calculated unit get temperature-dependent observed faility, the SLL and scattering cross sections were calculated unit get temperature-dependent of the scattering observed to the scattering of the scattering of the scattering of the scattering of the scattering observed to the scattering of the scattering of the scattering of the scattering observed to the scattering of the scattering observed to the scattering of the scattering observed to the sc

OS. Comparison with the results from the temperature-independent DOS obtained via AILD Be metal inflations revealed that the inelastic scattering cross sections differed by up to 20% at 1000 K.

I. Machine-learning potential: Spectral Neighbor Analysis Potential (SNAP) methodology [2]

to simulation data. Mischine-scarning morecular dynamics (MLOLD) was Societymany personance of ned MLP. To validate the accuracy of the final MLP, we calculated the phonon DOS from low-temp



\* AILD/MD: VASP code [3] \* MLMD: LAMMPS code [4] 2.3. Thermal scattering law (TSL) and cross section evaluation

2.3. Intermal scattering and (J.S.) and cross section evaluation
The TSL and the cross sections were evaluated using the Full Law Analysis Scattering System Hub (FLASSH) [5].

\* Based on the phonon DOS obtained from MLIAD using the trained SNAP model
The cubic approximation was applied, assuming isotropic phonon dispersion.
Natural intotypic compositions were assumed for beryllium and curbon.

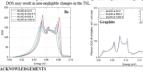
3.2. Temperature-dependent phonon DOS

NAPs were trained using AILD (Be metal) and AIMD (graphite) calculation data, with configuration MLMD was performed at such high temperatures using the trained SNAPs to calculate VACFs and the phonon

The characteristic peaks broaden, with their heights reduced

The DOS for acoustic phonon modes in the low-energy region deviates more and more from the DOS at 20 K.

Since the TSL is highly sensitive to the DOS in this region, this implies that using temperature-dependent

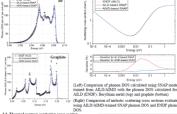


MD, have intrinsic limitations in accuracy

Can model materials at finite temperatures Applicable not only to crystalline solids but als

### 2 Parults

Deviations propagated to the inelastic scattering cross sections were less than a few % across the entire E s



3.3. Thermal neutron scattering cross section Using the temperature-dependent phonon DOS. also evaluated using the T-independent (ENDF:

All D-based) DOS at the same temperatures

 For Be metal and graphite, we trained SNAP models
 Comparison of inelastic scattering cross section evaluated using T-dependent and T-independent D used on data obtained from both AILD and AIMD simulations and verified the accuracy of the method as well as the trained SNAP models.

similations and verified the accuracy of the method as well as the trained SNAP models.

We successfully obtained temperature dependent planess DOS with an accuracy comparable to that of a do initio calculations. The impact of counséring temperature effects on the planon DOS was investigated, and one one-gligible defiremence was found in the neutraling thermal neutron accurance gross section data.

\*This method enables the evaluation of TSL data across a value range of temperatures with enhanced fidelity by acceptancing integratures depended phones DOS, infarth has relying on a single, temperature
for the properature depended phones DOS, infarth has relying on a single, temperature
strength of the properature depended phones DOS, infarth has relying on a single. Emperature-

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1. Machine-learning notential: Spectral Neighbor Analysis Potential (SNAP) methodology [2]



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Junhyoung Gil and Ayman I. Hawari

North Carolina State University, Department of Nuclear Engineering, 2500 Stinson Dr, Raleigh NC 27607, USA

ANSTRACT
The formal cuttering law (TSL) quartifies the node of energy and momentum transfer of low-energy neutrons white answerist. Accuse TSL data are thus executed for predesting a success reactive specification and solidy accusements. The contract transfer of low-energy neutrons in more raised and executed transfer of low-energy neutrons in an extractive transfer. To call the format is a contractive transfer of low-energy neutrons in more raised mentions. The contractive transfer of low-energy neutrons in more raised mentions. The contractive transfer of low-energy neutrons in more raised mentions. The contractive transfer of low-energy neutrons in more raised mentions. The contractive transfer of low-energy neutrons in more raised mentions. The contractive transfer of low-energy neutrons in more raised mentions. The contractive transfer of low-energy neutrons in more raised mentions. The contractive transfer of low-energy neutrons in more raised mentions. The contractive transfer of low-energy neutrons in more raised mentions. The contractive transfer of low-energy neutrons in more raised mentions. The contractive transfer of low-energy neutrons in more raised mentions. The contractive transfer of low-energy neutrons in more raised mentions. The contractive transfer of low-energy neutrons in more raised mentions. The contractive transfer of low-energy neutrons in more raised mentions. The contractive transfer of low-energy neutrons in more raised mentions. The photometric desirable and security predictions and contractive transfer of low-energy neutrons in more raised mentions and executive productive transfer of low-energy neutrons in more raised mentions and executive productive desirable and executive productive (LDLD). The desirable for executive productive desirable of the photometric desirable and executive productive desirable of the photometric desirable and executive productive (DDLD). The energy neutrons in more raised and instructive (DDLD) and instruments and instruments. The photometric desirab

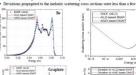
Machine-learning molecular dynamics (MLMD)

stated MLP to tasket the control of the final MLP are classically be placed to the control of the control of the final MLP are classically be placed to the control of the final solution scheding class schedules (MLP) and the period DOS observed resources of the final solutions calculated from the generated DOS observed from the control of the final solution of the solution of the final solution of the Trains a machine-learning potential to reproduce the energies, forces, and stress tensors of ab initio simus Enables sufficiently large system sizes and long simulation lengths within a reasonable computational time. Calculation of temperature-dependent phonon DOS of neutron moderator materials with near quantum mechanical accuracy by applying a machine-learning potentia

3. Results

3.1. Validation of the method SNAP was trained using AILD/AIMD data, with configurations sampled via MLMD at 20 K

Sover was named using ALLO ARADIA that said, with Configuration Surgices via statuto at a 30.
 MALMD was performed at 30 K using the trained SNAP to calculate VACF and the corresponding phonon in This phonon DOS was compared with the phonon DOS obtained via AILD to validate the overall method.
 A restoundle agreement was observed in the phonon DOS.
 Deviations propagated to the inelastic scattering cross sections were less than a few % across the entire E in the property of the property o



From this short MLMD, the

\* AILD/MD: VASP code [3] \* MLMD: LAMMPS code [4] And a terminal recentage and (13 kL) also cross section in ratioation.

The TSL and the cross sections were evaluated using the PLI Law Analysis Scattering System Hub (FLASSH) [S]

8 Based on the phonon DOS obtained from MLADD using the trained SNAP model.

The cubic approximation was applied, assuraning isotropic phonon dispersion.

Nothinal isotopic compositions were assumed for beryllium and carbon.

and used to perform MLMD for a short duration.

configuration space is

explored and sampled.

AILD MD simulations are

AILD-training' sequence

3.2. Temperature-dependent phonon DOS NAPs were trained using AILD (Be metal) and AIMD (graphite) calculation data, with configurations sampled MLMD was performed at such high temperatures using the trained SNAPs to calculate VACFs and the phonon

Sample

(s=0) Train

The n-th version of SNAP

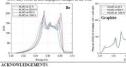
toot: Finish

NAP-MLMD to produce VACF

2.3. Thermal scattering law (TSL) and cross section evaluation.

The DOS for acoustic phonon modes in the lone-energy region deviates more and more from the DOS at 20 K.

Since the TSL is highly sensitive to the DOS in this region, this implies that using temperature-dependent DOS may result in non-neighble changes in the TSL.



(Left) Comparison of phonoco DOS calculated using SNAP mode trained from AlLD/AlMD with the phonon DOS calculated from AlLD (ENDF): Beryllium metal (top) and graphite (bottom) (Right) Comparison of inelastic scattering cross sections eval

also evaluated using the T-independent (ENDF) AILD-based) DOS at the same temperatures

At 1200 K, the cross section derived from

We established and validated a metho evaluating temperature-dependent phonon DOS using MLMD simulations.

 For Be metal and graphite, we trained SNAP models based on data obtained from both AILD and AIMD

simulations and verified the accuracy of the method as well as the trained SNAP models.

We successfully obtained temperature-dependent phonon DOS with an accuracy comparable to that of ab initio calculations. The impact of considering temperature effects on the phonon DOS was investigated, an one-negligible difference was found in the resulting thermal neutron scattering cross section data.

This method enables the evaluation of TSL data across a wide range of temperatures with enhanced fidelit by incorporating temperature-dependent phonon DOS, rather than relying on a single, temperature-



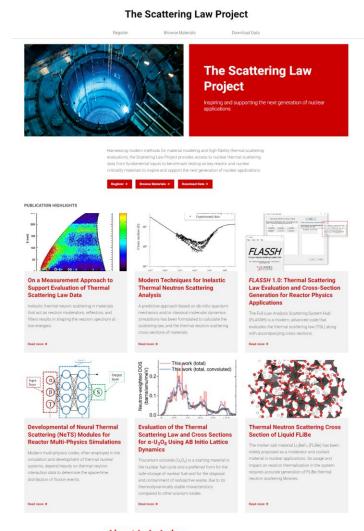
### Summary

- Advanced nuclear reactors represent an excellent opportunity for innovation
  - Revived our knowledge of fundamental radiation interaction physics
  - Allowed the introduction of modern methods
    - computational and experimental
- Integration of computation and experimentation to see the unseen
  - Hybrid and adaptive
- Innovation is great for mentoring the next generation of nuclear engineering and science experts



### **TSL Project**

- ☐ TSL Project website will be launched at **TAMU** during Fall 2025
- Will be include all LEIP work
  - ☐ TSL files (File 7)
  - ACE files
  - NeTS
  - Benchmark and validation work
  - All published work (papers, reports, PhD and MS theses, etc.)
- Will be open to all
  - Request feedback from users



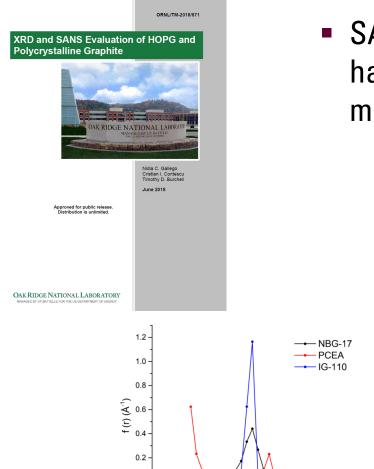


## Thank You



### What Else?

### **SANS Observations**

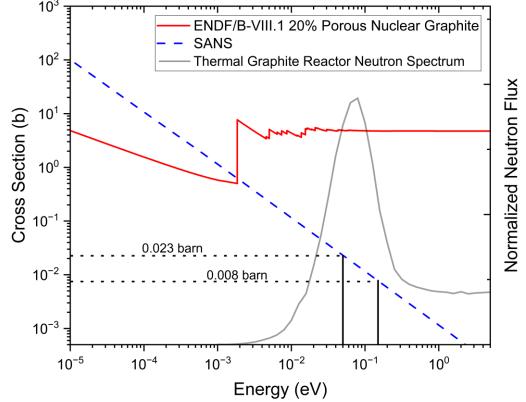


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r(Å)

Figure 18 (b) from Reference

 SANS contributions, based on data from the reference below, have a <u>negligible impact</u> on the total cross section and do not modify neutron thermalization in a reactor.

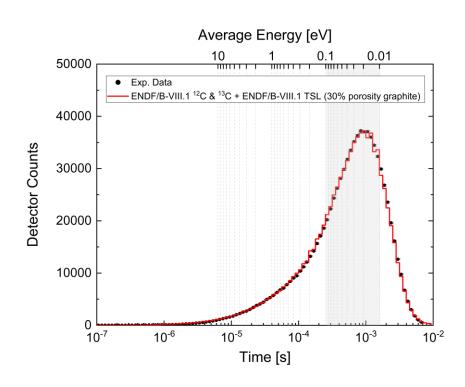


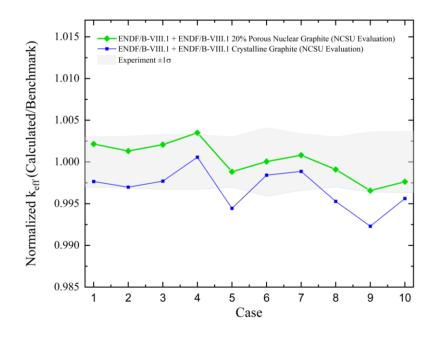
Ref. 2 - Petriw, et.al., "Porosity effects on the neutron total cross section of graphite"

### **Graphite Density**

ORELA and PROTEUS with porous nuclear graphite density (i.e. use 1.6-1.7 g/cm³)

**Self-consistent** phonon DOS and density



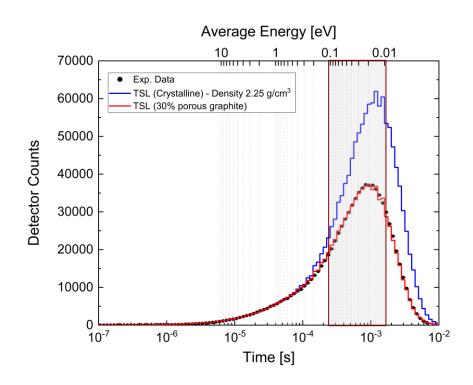


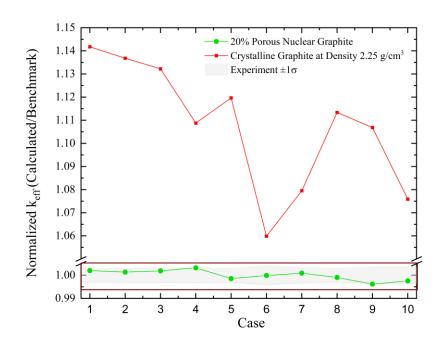


### **Graphite Density**

ORELA and PROTEUS without historical density approximation (i.e. use 2.25 g/cm³)

**Self-consistent** phonon DOS and density



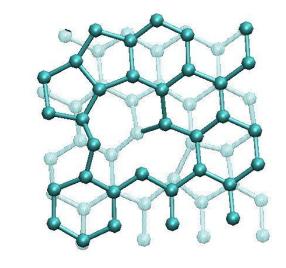




### **Radiation Damage Interplanar Di-vacancy Defect**

Observed in the MD system following cascade sequence. MD is predictive in this sense because no a-priori assumptions are necessary regarding the defect structure.

Static *ab-initio*, on the other hand, requires some initial guess that is then subject to optimization.



Development of the Thermal Neutron Scattering Cross Sections of Graphitic Systems using Classical Molecular Dynamics Simulation

Brian Douglas Hehr

A dissertation submitted to the Graduate Faculty of North Carolina State University in partial fulfillment of the equirements for the Degree of

Nuclear Engineering

Raleigh, North Carolina

APPROVED BY

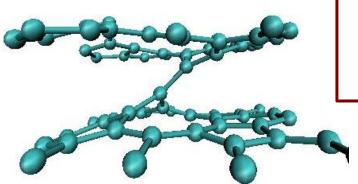
Dr. Mohamed A. Bourham

Dr. Albert R. Young

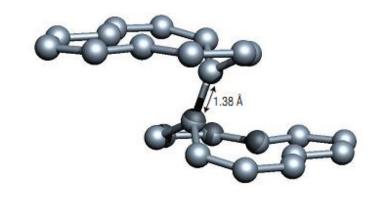
Dr. Ayman I. Hawari,

Dr. Bernard W. Wehring

Chair of Advisory Committe



LEIP MD analysis



R. H. Telling, C. P. Ewels, A. A. El-Barbary and M. I. Heggie. Nature Materials. 2, 333 (2003). (ab-initio)

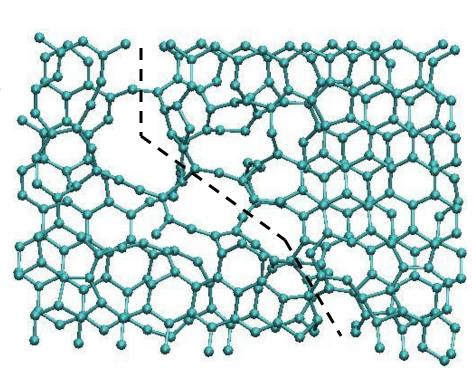


# Radiation Damage Interplanar Crosslinking

With increasing cascade buildup, the basal planes of graphite cross-link.

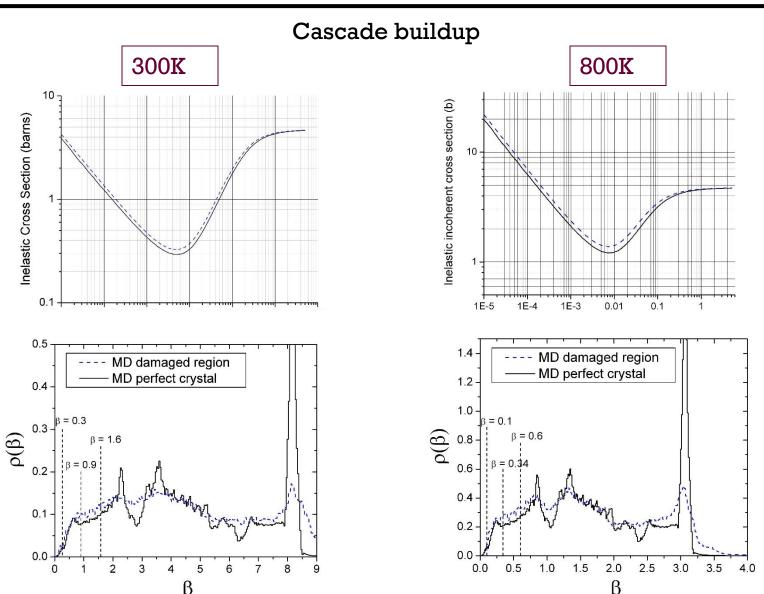
distinguishable

→ Individual point defects become less





### Radiation Damage Effect of Temperature



Porosity
effect
continues
to dominate

