Development and Verification of the Thermal Scattering Cross-section Calculation Module ThermaIXS in AXSP

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Abstract

Based on neutron thermal scattering theory, this work first developed a neutron thermal scattering cross-section calculation module, ThermalXS, in the self-developed evaluated nuclear data processing program AXSP. Utilizing thermal scattering law files for nuclides such as U, H, and Zr, various types of neutron thermal scattering cross-sections were calculated and compared with results from the THERMR module of the NJOY2016 program, thereby verifying the correctness of ThermalXS for thermal neutron calculations. Compared with the THERMR module, ThermalXS employs adaptive incident energy grid technology, which ensures more accurate thermal scattering cross-sections for metal hydrides, and can process thermal scattering rate data with one-phonon corrections. This paper analyzes and compares the variations in graphite thermal scattering cross-sections among the ENDF/B-VII.1, ENDF/B-VIII.0, and ENDF/B-VIII.1 evaluated nuclear data libraries, and compares them with experimental values. The study finds that: the graphite thermal scattering cross-sections in the latest ENDF/B-VIII.1, which introduces non-cubic formulas and one-phonon corrections, show better agreement with experimental values than those using the incoherent approximation; the calculated reactor graphite thermal scattering cross-sections in ENDF/B-VIII.1 exhibit a trend of increasing with porosity, but remain significantly smaller than experimental data for porous graphite, indicating that the functionality of the thermal scattering data generation module requires further improvement.

Full Text

Development and Verification of the Thermal Scattering Cross Section Calculation Module ThermalXS in AXSP

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Abstract

This work first developed a neutron thermal scattering cross-section calculation module, ThermalXS, in the independently developed evaluated nuclear data processing program AXSP based on neutron thermal scattering theory. The module calculated different types of neutron thermal scattering cross-sections using thermal scattering law files for nuclei such as U, H, and Zr, and verified the correctness of the ThermalXS module for thermal neutron calculations by comparing the results with those from the THERMR module in the NJOY2016 program. Compared with the THERMR module, ThermalXS employs an adaptive incident energy grid technology that ensures more accurate thermal scattering cross-sections for metal hydrides, and ThermalXS can process one-phonon-corrected thermal scattering law data.

This paper analyzes and compares the changes in graphite thermal scattering cross-sections in the ENDF/B-VII.1, ENDF/B-VIII.0, and ENDF/B-VIII.1 evaluated nuclear databases and compares them with experimental values. The study finds that the latest ENDF/B-VIII.1, which introduces a non-cubic formula and one-phonon correction for graphite thermal scattering cross-sections, shows better agreement with experimental values compared to cross-sections using the incoherent approximation. The calculated reactor graphite thermal scattering cross-sections in ENDF/B-VIII.1 exhibit a trend of increasing with porosity, but are still far smaller than experimental data for porous graphite, indicating that the functionality of the thermal scattering data generation module needs further improvement.

Keywords: Neutron thermal scattering; Double-differential scattering cross-section; ThermalXS; Reactor grade graphite

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With the rapid development of nuclear reactor technology both domestically and internationally, the requirements for practical application calculations in nuclear reactors have also increased. In the process of reactor physics calculations, neutron scattering in various energy regions must be considered, among which thermal neutron scattering corresponding to the thermal energy region has significant impacts on reactor safety design, neutron transport calculations, and critical safety analysis [**?**]. For example, thermal neutron scattering dominates the positive temperature effect in materials such as zirconium hydride and lithium hydride [**?**]. When neutrons are in the thermal energy region, scattering between neutrons and target nuclei becomes complex due to thermal motion of target nuclei, interference effects of scattering waves, and chemical bonding, leading to calculations of secondary neutron energy and angular distributions and scattering cross-sections that require consideration of additional factors [**?**]. With the proposal of concepts such as numerical reactors, nuclear reactor design has demanded higher precision for thermal neutron scattering cross-sections. Due to graphite' s excellent neutron moderation properties, it has been widely applied in fourth-generation reactor designs such as molten salt reactors and high-temperature gas-cooled reactors. High-precision graphite thermal neutron cross-sections have important impacts not only on reactor physics calculations but also on reactor safety, making it necessary to conduct research on high-precision thermal neutron cross-sections for graphite.

Since the 1960s, extensive research has been conducted on thermal neutron scattering cross-sections both domestically and internationally, and many thermal neutron cross-section processing software programs have been developed, such as FLASSH developed by the Nuclear Engineering Department of North Carolina State University [**?**], HEXSCAT developed by General Atomic Company [**?**], FLANGE-II developed by Savannah River National Laboratory [**?**], and NJOY developed by Los Alamos National Laboratory [**?**]. Domestic research on evaluated nuclear data processing programs has also been thorough, such as NECP-Atlas developed by Xi' an Jiaotong University [**?**], RXSP developed by Tsinghua University [**?**], Ruler developed by China Institute of Atomic Energy [**?**], and the advanced nuclear data processing software AXSP developed by North China Electric Power University [**?**]. This paper first conducted in-depth research on neutron thermal scattering theory, then further improved the calculation functions of the thermal scattering cross-section calculation module ThermalXS in AXSP using Fortran2003 with object-oriented programming. The accuracy of ThermalXS calculations was verified by comparing with calculation results from the NJOY-THERMR module. Based on the thermal neutron scattering law data for graphite in the ENDF/B-VII.1, ENDF/B-VIII.0, and ENDF/B-VIII.1 libraries, the thermal scattering cross-sections calculated by ThermalXS were compared with experimental results to obtain the effects of different databases and thermal scattering law data with different porosities on graphite thermal scattering cross-sections. It was found that the calculation results of the thermal scattering files introduced in ENDF/B-VIII.1 with one-phonon correction have significantly improved accuracy compared to previ-

ous versions and show good agreement with Steyerl' s polycrystalline graphite experimental data, demonstrating that introducing one-phonon correction can effectively improve errors introduced by the incoherent approximation. Comparing ENDF/B-VIII.1 reactor graphite with 10%, 20%, and 30% porosity, it was found that graphite thermal scattering cross-sections increase with increasing porosity, but the calculated thermal scattering cross-sections below 10^{-2} eV are still far smaller than experimental data for graphite with porosity.

1 Neutron Thermal Scattering Cross Section Calculation Theory

Currently, three main types of thermal scattering cross-sections are considered domestically and internationally: incoherent inelastic scattering, incoherent elastic scattering, and coherent elastic scattering [**?**]. The theoretical models for these three types of scattering cross-sections are introduced below.

1.1 Thermal Neutron Scattering Law

In reactor physics, fast neutrons produced by fission become thermal neutrons after moderation. Since thermal neutron energy is close to target nucleus energy, scattering is influenced by thermal motion of scattering nuclei, interference effects of scattering waves, and chemical bonding, resulting in complex scattering. These effects are closely related to the crystal and molecular properties of the target material itself. The ENDF/B evaluated nuclear data describes the scattering properties of different materials with neutrons in the thermal energy region using thermal scattering law data (TSL) in File 7.

Thermal scattering law data is divided into three types: $S(\alpha, \beta, T)$ is the thermal scattering law data in ENDF that describes incoherent inelastic scattering. Since thermal neutrons undergo incoherent inelastic scattering with various target materials, $S(\alpha, \beta, T)$ is present in every thermal scattering law file. For hydrogen-containing solid materials such as ZrH, solid methane, and polyethylene, incoherent elastic scattering must be considered [**?**], which ENDF describes using the Debye-Waller factor $W(T)$. For crystalline materials such as graphite, BeO, UO_2, and SiO_2, coherent elastic scattering must be considered due to Bragg diffraction, requiring the use of $S(E, T)$. Currently, thermal scattering law data in the ENDF/B-VIII.1 library is mainly generated by the NJOY-LEAPR program and the FLASSH program.

1.2 Incoherent Inelastic Scattering

The double-differential scattering cross-section formula for incoherent inelastic scattering is:

$$\frac{d^2\sigma}{dE'd\Omega} = \frac{\sigma_b}{4\pi}\sqrt{\frac{E'}{E}}\frac{1}{kT}\sum_{n=1}^{N_S} M_{nS} n(\alpha, \beta, T) e^{-\beta/2}$$

where σ_b is the scattering cross-section; N_S is the number of non-principal scattering atom types; k is the Boltzmann constant; T is temperature in K; E' is secondary neutron energy (eV), E is incident neutron energy (eV); μ is the scattering angle cosine (in laboratory frame); M_n is the number of the nth type of atom in the target material; $S_n(\alpha, \beta, T)$ represents the scattering function corresponding to the scattering law data, which can be read from File 7 when calculating equation (1); σ_{bn} is the characteristic incoherent cross-section of the nth target nucleus in the material; α and β are dimensionless quantities representing the momentum transfer and energy transfer of the neutron, respectively, characterizing the changes in neutron angle and energy before and after scattering [**?**]. The specific expressions for α, β, and σ_{bn} are:

$$\alpha = \frac{(E' + E - 2\sqrt{EE'}\mu)}{AkT}$$

$$\beta = \frac{(E' - E)}{kT}$$

$$\sigma_{bn} = \sigma_{fn}\frac{(A_n + 1)^2}{A_n^2}$$

where A_0 is the mass of the principal scattering atom in the molecule; σ_{fn} is the free-atom scattering cross-section of the nth type of atom; A_n is the mass ratio of the nth type of atom to the neutron mass.

In actual calculations, since interpolation of scattering law data is required and $S_n(\alpha, \beta, T)$ corresponds to a specific temperature T, when the incident neutron energy is too high, α and β may exceed the values provided for $S_n(\alpha, \beta, T)$ in File 7. In this case, $S_n(\alpha, \beta, T)$ cannot be read from File 7, and the short collision time (SCT) approximation must be used to obtain $S_n(\alpha, \beta, T)$. The calculation formula is:

$$S_{SCT}(\alpha, \beta, T) = \frac{1}{\sqrt{4\pi\alpha T_{eff}/T}} \exp\left[-\frac{(\beta - \alpha)^2}{4\alpha T_{eff}/T}\right]$$

where T_{eff} is the effective temperature, with specific values given in File 7, and other symbols have the same meaning as in previous formulas. Although ENDF-format scattering law data includes data for many common materials, scattering law data is not provided for most nuclides. For thermal scattering cross-section calculations of these nuclides without scattering law data, the free gas model can generally be used as an approximation, assuming that neutrons scatter with target nuclei and all atomic nuclei are in free thermal equilibrium motion without being bound by chemical bonds. Using the free gas model to calculate the double-differential scattering cross-section, the calculation formula

is similar to (1.1), except that $S_n(\alpha, \beta, T)$ needs to be calculated separately without reading data from File 7. The calculation formula for $S_n(\alpha, \beta, T)$ is:

$$S_n(\alpha, \beta, T) = \frac{1}{\sqrt{4\pi\alpha}} \exp\left[-\frac{(\alpha-\beta)^2}{4\alpha}\right]$$

Additionally, when calculating the double-differential scattering cross-section using the free gas model, the elastic scattering cross-section of neutrons is typically considered constant, which leads to reduced calculation accuracy for some non-gaseous or crystalline materials.

1.3 Incoherent Elastic Scattering

An elastic scattering component exists in hydrogen-containing solids. When thermal neutrons collide with materials such as polyethylene and ZrH , incoherent elastic scattering occurs, which can be treated using the incoherent approximation. ENDF provides the double-differential cross-section formula for incoherent elastic scattering as:

$$\frac{d^2\sigma}{dE'd\Omega}(E \to E', \mu) = \frac{\sigma_b}{4\pi}\sqrt{\frac{E'}{E}}e^{-2W'(E-E')}\delta(\mu-\mu_0)$$

where σ_b is the characteristic scattering cross-section and W' is the Debye-Waller factor (eV^{-1}).

1.4 Coherent Elastic Scattering

When considering scattering reactions between crystalline materials and thermal neutrons, due to the special structure of crystals, the scattering exhibits diffraction properties, making coherent elastic scattering particularly important. Its double-differential cross-section formula is:

$$\frac{d^2\sigma}{dE'd\Omega}(E \to E', \mu) = \frac{1}{2E}\sum_i s_i\delta(\mu-\mu_i)\delta(E-E_i)$$

where E_i is the ith Bragg edge less than the incident energy E; s_i is proportional to the structure factor; μ_i is the characteristic scattering angle cosine for each crystal plane, expressed as:

$$\mu_i = 1 - \frac{2E_i}{E}$$

When calculating the double-differential cross-section for coherent elastic scattering, the formula can be simplified as:

$$\sigma(E,\mu) = \sum_i \frac{s_i}{2E}\delta(\mu - \mu_i)$$

In actual calculations, $S(E,T)$ can be obtained from File 7. For incident energy values, the incident energy data regarding elastic scattering in File 3 of the ENDF file can be read. When the incident energy is determined, according to equations (10) and (9), the outgoing energy and scattering angle cosine are also determined, so equation (10) can be simplified as:

$$\sigma(E) = \sum_i \frac{s_i}{2E}$$

From equation (11), it can be seen that the calculated value of the coherent elastic scattering cross-section is equivalent to the calculated value of the double-differential coherent scattering cross-section.

2 Program Development

2.1 Program Overview

Based on the three thermal neutron scattering calculation formulas and using the Fortran2003 language with object-oriented programming concepts, the thermal scattering cross-section data processing module ThermalXS was developed. This program possesses the main functions of the THERMR module in NJOY and can calculate and generate the required thermal scattering cross-section data for reactor calculations based on the scattering law data provided in File 7 of ENDF and the properties of different nuclides, thereby further improving the functionality of the AXSP software.

2.2 Program Design

First, the data in File 7 is read, classified, and interpolated according to different nuclides and scattering types. For the free gas model, since no data reading is required, the value of $S(\alpha,\beta)$ is first calculated in the program. Before solving for $S(\alpha,\beta)$, α and β must be calculated in advance. According to equations (1) and (3), α and β are related to incident energy, outgoing energy, and scattering angle cosine. For incident energy values in the program, an energy grid is generally divided. Considering that incident neutrons are in the thermal energy region, 118 energy points are divided from low to high, with the minimum set at 1×10^{-5} eV and the maximum at 4 eV. Simultaneously, β is also divided into a grid of 45 values from low to high, with a minimum of 0 and a maximum of 3500. For the scattering angle cosine, the inverted stack method is used, substituting μ from the interval (-1,1) into equation (6), and combining it with the previously divided incident energy and β grids to obtain values for α and outgoing energy. The values obtained from each μ inversion are recorded, ultimately yielding a linear relationship between μ and $S(\alpha,\beta)$. Based on this linear

relationship, Gaussian-Legendre integration is performed on equation (1) with respect to μ to obtain the differential cross-section $\sigma(E, E')$. Then $\sigma(E, E')$ is integrated using the trapezoidal rule with respect to E' under each incident energy point to obtain the incoherent inelastic cross-section $\sigma(E)$ under the free gas model. Since the final scattering probability density needs to be generated, the scattering probability $P(E \to E')$ must also be calculated using the formula:

$$P(E \to E') = \frac{\sigma(E \to E')}{\sigma(E)}$$

For nuclides with File 7 data, after reading the data, interpolation is performed on $S_n(\alpha, \beta, T)$, α, and β, so no β grid division is needed, but the incident energy grid division is consistent with the free gas model. After completing data interpolation, the corresponding formulas are substituted according to different scattering types to obtain the corresponding scattering cross-sections. The specific interpolation process, interpolation method, and integration process are similar to the free gas model and will not be elaborated further. Finally, the calculated cross-section data is processed into PENDF format files and then output into ACE format files for practical use.

Following the above steps, the main operational framework of ThermalXS is shown in Figure 1 [Figure 1: see original paper].

2.3 Program Numerical Verification

Using the ThermalXS program to calculate thermal scattering cross-sections at 296 K temperature and comparing with calculation results from the NJOY-THERMR program, the coherent elastic scattering cross-section and incoherent inelastic scattering cross-section of ^{235}U in UO_2 are shown in Figures 2 [Figure 2: see original paper] and 3 [Figure 3: see original paper], the incoherent inelastic scattering cross-section of ^{1}H in H_2O is shown in Figure 4 [Figure 4: see original paper], and the incoherent elastic scattering cross-section of H in ZrH is shown in Figure 5 [Figure 5: see original paper]. The incoherent elastic scattering cross-section values of ^{235}U in UO_2 calculated using the free gas model are shown in Figure 6 [Figure 6: see original paper]. The results show good agreement between ThermalXS and NJOY calculations, ensuring the accuracy of the program calculations. The calculation results of the ThermalXS module are stored in pendf format in files, which can be used by the subsequent GroupXS module to calculate multi-group cross-section constants based on two-body and many-body dynamics [**?**].

Compared with the THERMR module in the NJOY program, the ThermalXS module implements adaptive changes to the incident energy grid. The THERMR module uses a built-in fixed energy grid of 118 points for thermal scattering cross-section calculations, which has poor calculation accuracy and cannot accurately reflect the oscillation phenomena of incoherent inelastic scattering when processing metal hydrides. ThermalXS establishes an adaptive

energy grid based on the dimensionless energy transfer β grid contained in the inelastic scattering thermal scattering law data $S(\alpha, \beta)$. The adaptive energy grid is denser than the fixed energy grid and is material-dependent. The metal hydride incoherent inelastic scattering cross-sections calculated by the ThermalXS program show clear oscillations. The comparison between calculation results from the THERMR module and the ThermalXS module is shown in Figure 7 [Figure 7: see original paper].

3 Analysis of ENDF/B Thermal Scattering Law Libraries and Related Experiments

3.1 Changes in ENDF/B Thermal Scattering Law Libraries and Introduction to Related Experiments

Graphite moderator plays an important role in the design and construction of new-generation reactors. Researchers both domestically and internationally are committed to developing more accurate graphite thermal scattering data, and the ENDF/B evaluated nuclear database continuously updates and improves graphite thermal scattering law files. The ENDF/B-VII.1 library contains only one graphite thermal scattering law file, while the ENDF/B-VIII.0 evaluated nuclear database includes three graphite thermal scattering law files, divided into crystalline graphite, reactor graphite with 10% porosity, and reactor graphite with 30% porosity. All these thermal scattering law files are calculated and generated by the NJOY-LEAPR module.

The latest ENDF/B-VIII.1 version adds graphite thermal scattering law data files considering one-phonon correction and non-cubic models, as well as reactor graphite with 20% porosity, generated using the FLASSH (Full Law Analysis Scattering System Hub) program [**?**]. The non-cubic formula is a prerequisite for implementing one-phonon correction. The relevant experimental information used for comparison with thermal scattering cross-section calculation results is shown in Table 1 . The experimental data comes from the EXFOR database, where X4 indicates the data number in the database.

Table 1 Relevant experimental data information

EXFOR Number	Sample Density (g/cm^3)	Porosity (%)	Test Temperature (K)
Steyerl 1			
Steyerl 2			
Bowman			
Robledo			

In 1965, Neil et al. experimentally measured the thermal scattering cross-section of polycrystalline graphite samples in the energy region above 10^{-3} eV. In 1974, Steyerl et al. conducted two experiments using polycrystalline graphite and a

neutron bottle [**?**]. To avoid confusion in the following text, the polycrystalline graphite experiment is referred to as Steyerl1 and the neutron bottle experiment as Steyerl2. The Steyerl1 experiment was conducted at 295 K using polycrystalline graphite 3.8 mm thick with a density of 2.24 g/cm^3, and the experimental data mainly concentrated in the energy region below 10^{-3} eV. The neutron bottle experiment used columnar electro-graphite coated with a uniform, porous, high-purity pyrolytic graphite layer of 2-3 m thickness, with a column density of 1.715 g/cm^3 and a coating density of 2.05 g/cm^3.

The Bowman experiment [**?**] involved filling powdered graphite with an average density of 1.03 g/cm^3 into a tank 8 feet in diameter and 8 feet high for scattering experiments. Since the graphite sample was crushed, precise porosity could not be calculated. The reason for selecting this experiment is that graphite materials used in high-temperature gas-cooled reactor construction include not only bulk graphite reflectors but also graphite powder loaded in fuel boxes. Comparing Bowman' s powdered graphite experiment with program calculation values has certain practical significance for gas-cooled reactor research. In 2020, J.I. Robledo [**?**] et al. at CAB used the VESUVIO time-of-flight spectrometer to measure the total cross-section of isostatically pressed graphite samples. The graphite sample used was mentioned in a 2010 CAB article studying the effect of porosity on graphite total cross-section. The graphite sample weighed 196.8 g with a density of 1.740 g/cm^3, and the porosity was calculated to be approximately 23% [**?**].

3.2 Comparative Analysis of Crystalline Graphite Thermal Scattering Cross-Sections from ENDF/B-VII.1, ENDF/B-VIII.0, and ENDF/B-VIII.1 Libraries with Experimental Values

Compared with the ENDF/B-VII.1 evaluated nuclear database, the ENDF/B-VIII.0 evaluated nuclear database established a new graphite model by North Carolina State University (NCSU), using advanced ab initio lattice dynamics (AILD) to calculate the phonon density of states for crystalline graphite [**?**]. Using the phonon density of states as input, the NJOY-LEAPR module calculates the thermal scattering law data for crystalline graphite (tsl-crystalline-graphite).

The ENDF/B-VIII.1 version evaluated nuclear database uses the FLASSH (Full Law Analysis Scattering System Hub) program to generate graphite thermal scattering law files considering one-phonon correction and non-cubic models (tsl-graphiteSd) and reactor graphite files with 20% porosity (tsl-reactor-graphite-20P), eliminating errors introduced by the incoherent approximation and cubic approximation. Based on the ENDF/B-VII.1, ENDF/B-VIII.0, and ENDF/B-VIII.1 evaluated nuclear databases [**?**], the calculated inelastic scattering cross-sections for graphite at 296 K temperature are shown in Figure 8 [Figure 8: see original paper].

Figure 8 Comparison of graphite thermal scattering cross-sections with one-phonon correction, crystalline graphite thermal scattering cross-sections, and

experimental values (color online)

As shown in Figure 8, the crystalline graphite inelastic scattering cross-sections from ENDF/B-VIII.0 and ENDF/B-VIII.1 are basically the same and slightly higher than the crystalline graphite thermal scattering cross-section from ENDF/VII.1. This is because the phonon density of states used in the evaluation of crystalline graphite thermal scattering law data in ENDF/B-VIII.0 and ENDF/B-VIII.1 is calculated using the first-principles method of ab initio lattice dynamics (AILD), which can more accurately simulate the crystalline properties of materials, making the calculated cross-sections closer to experimental values. However, the above three sets of cross-sections are still smaller than experimental values because graphite crystals are non-cubic crystals with anisotropic interatomic forces. The LEAPR program used in thermal scattering law data calculation employs cubic approximation and incoherent approximation, which introduce significant errors in the calculation of graphite thermal scattering law and thermal scattering cross-sections. The graphite inelastic scattering cross-section calculation results from ENDF/B-VIII.1 introducing the non-cubic formula and one-phonon correction are significantly higher than previous versions and show good agreement with Steyerl1 experimental data, demonstrating that removing the incoherent approximation and cubic approximation is important for accurately calculating cross-sections of anisotropic crystals such as graphite.

3.3 Comparison of Thermal Scattering Cross-Sections for Reactor Graphite with Different Porosities in ENDF/B-VIII.1 Library

In research, it was found that graphite porosity causes the measured total cross-section of graphite in the low-energy region to be greater than the theoretically calculated total cross-section. Therefore, starting from ENDF/B-VIII.0, thermal scattering law files for reactor graphite with porosity were added. The phonon density of states for crystalline graphite is calculated using ab initio lattice dynamics (AILD) based on first principles, while the phonon density of states for reactor graphite is calculated using classical molecular dynamics (MD). The porosity simulation method involves randomly removing atoms from the crystal structure to generate the phonon density of states, which is then used to calculate thermal scattering law data. As described in section 3.1, compared with ENDF/B-VII.1, the ENDF/B-VIII.0 evaluated library added reactor graphite with 10% porosity (tsl-reactor-graphite-10P) and reactor graphite with 30% porosity [**?**] (tsl-reactor-graphite-30P), while the ENDF/B-VIII.1 evaluated library added reactor graphite with 20% porosity (tsl-reactor-graphite-20P).

To study the effects of thermal scattering law data with different porosities on thermal neutron scattering cross-sections, this paper uses the ThermalXS program to read the thermal scattering law data for crystalline graphite, reactor graphite with 10% and 30% porosity from the ENDF/B-VIII.0 and ENDF/B-VIII.1 thermal scattering law libraries, and reactor graphite with 20% porosity from ENDF/B-VIII.1, and calculates the total thermal neutron scattering cross-

sections. The comparison of thermal neutron scattering cross-sections with different porosities and experimental values is shown in Figure 9 [Figure 9: see original paper].

Figure 9 Comparison of thermal scattering cross-sections for porous reactor graphite with experimental values (color online)

As shown in Figure 9, the thermal scattering cross-sections calculated from graphite thermal scattering law files with the same name in ENDF/B-VIII.0 and ENDF/B-VIII.1 are basically equal. Below the first Bragg peak, the magnitude relationship of the total thermal scattering cross-sections calculated by ThermalXS is: 30% reactor graphite > 20% porosity reactor graphite > 10% porosity reactor graphite > crystalline graphite, indicating that the thermal scattering law files in the ENDF/B evaluated library can already reflect the trend of thermal scattering cross-sections increasing with porosity. At and beyond the first Bragg peak, the total thermal scattering cross-section includes contributions from both inelastic and elastic scattering, and all calculated thermal scattering cross-section results can be seen to basically coincide. The calculation process for porous and non-porous graphite cross-sections is the same and does not require special treatment.

Comparing the calculation results with experimental values reveals that Neil' s crystalline graphite experimental results are mainly distributed in the energy range at and beyond the first Bragg peak, showing good agreement with the total thermal scattering cross-section calculated by ThermalXS. The graphite samples used in the Steyerl2, Bowman, and Robledo experiments have porosity. The Robledo experimental sample has a porosity of 23.2%, and the Bowman experiment [**?**] used powdered graphite, which, although its exact porosity cannot be calculated, can still be considered porous (see section 3.1 for specific experimental parameters). The experimental data from these two groups are much larger than the ThermalXS thermal scattering cross-section calculation results in the energy region below 0.01 eV. Below 0.0018 eV, the total cross-section equals the inelastic scattering cross-section, and between 0.0018 eV and 0.01 eV, the total cross-section is mainly contributed by coherent elastic scattering, indicating that the inelastic scattering law data and coherent elastic scattering law data in the porous graphite thermal scattering law files of the ENDF/B evaluated library cannot accurately evaluate the cross-sections of porous graphite.

The reason why increased porosity leads to increased graphite thermal scattering cross-section is that the pores of various sizes in reactor graphite are filled with air. Neutrons undergo refraction when passing through many solid/air interfaces in porous graphite, and more pores result in more small-angle scattering than in pure crystalline graphite, ultimately leading to increased total cross-section. However, current methods and models for thermal scattering law and thermal scattering cross-section calculations cannot fully simulate the effects of air/solid interfaces on scattering, indicating that the functionality of thermal scattering data calculation programs needs further improvement. The significant differences between the experimental results of Steyerl2, Bowman,

and Robledo and the evaluated database below 0.0018 eV may be related to porosity, and the specific reasons require further research.

4 Conclusions

Based on neutron thermal scattering theory and using the Fortran2003 language with object-oriented programming, this paper developed the thermal scattering cross-section processing program ThermalXS in the AXSP program. Based on the thermal scattering law data for ^{235}U in UO_2, H in H_2O, and H in ZrH from the ENDF/B-VII.1 evaluated nuclear database, the corresponding thermal scattering cross-sections were calculated and compared with calculation results from the NJOY program, proving that the thermal neutron scattering cross-sections obtained by ThermalXS are correct and have high precision. ThermalXS also employs an adaptive incident energy grid, which can better describe the fluctuation phenomena of metal hydride inelastic scattering cross-sections compared to NJOY' s fixed energy grid.

On this basis, the ThermalXS program was used to comprehensively calculate the graphite thermal scattering law files in the ENDF/B-VII.1, ENDF/B-VIII.0, and ENDF/B-VIII.1 evaluated nuclear databases, and horizontal comparisons within the same version, vertical comparisons between different versions, and comparisons between calculated values and experimental values were conducted, leading to the following conclusions:

The inelastic scattering cross-section values calculated based on the graphite thermal scattering law files in ENDF/B-VIII.1 that introduce the non-cubic formula and one-phonon correction show a significant increase in the low-energy region compared to crystalline graphite cross-sections that introduce the incoherent approximation and cubic approximation, and show good agreement with experimental values. This proves that using the non-cubic formula and one-phonon correction to eliminate non-cubic approximation and incoherent approximation can effectively improve the accuracy of crystalline graphite thermal scattering law data. Currently, no other domestic units have calculated and verified the ENDF/B-VIII.1 graphite thermal scattering law files, and this work can provide a reference for related domestic research.

The ThermalXS program calculation results show the magnitude relationship of graphite thermal scattering cross-sections as: 30% porosity reactor graphite $>$ 20% porosity reactor graphite $>$ 10% porosity reactor graphite $>$ crystalline graphite, indicating that graphite thermal scattering cross-sections increase with increasing porosity. However, the calculated thermal scattering cross-sections below 10^{-2} eV are still far smaller than experimental data for reactor graphite with porosity, indicating that current methods and models for thermal scattering law calculation cannot fully simulate the effects of air/solid interfaces in pores on scattering, and the functionality of thermal scattering data generation modules needs further improvement.

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Note: Figure translations are in progress. See original paper for figures.