Physics AUC, vol. 29, 45-49 (2019) **PHYSICS AUC**

Generation of thermal scattering cross sections for Sapphire (Al_2O_3) and Bi Crystal filters used in nuclear facilities

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Abstract

Sapphire and Bismuth crystals are used as fast neutrons and high energy gammas filters for several nuclear facilities such as Prompt Gammas Activation facility, Neutron diffraction, Neutron Imaging around research reactors. In this paper, we will focus on phonon frequency distributions (density of states) generation. As a tool, we used the ifit mccode, PhonoPy and Quantum-expresso package. The obtained information's were enfolded in LEAPR module of the NJOY 2016 code to prepare the scattering law $S(\alpha, \beta)$ at various temperatures.

KEYWORDS: Neutron, Thermal Neutron, Phonon Frequency Distribution, Scattering Law S(A, B), Sapphire, Bismuth

Introduction

In MCNP package, the cross section data do not take of consideration the structure of material. However, the mt card can be used for correction the cross section at thermal energy. This data was processed by LEAPR module using NJOY [2]. The LEAPR module was used to calculate the thermal inelastic scattering cross section for Sapphire and Bismuth with only user can defined data for a phonon frequency spectrum. The Thermal inelastic scattering is important for all materials. The cross sections for thermal neutrons are calculated from the exact shape of the phonon frequency spectrum. The thermal scattering law is a function of two non-dimensional quantities, momentum exchange variable α and energy exchange variable β.

$$\alpha = \frac{E - E' + 2\mu\sqrt{E'E}}{Ak_BT} \; ; \beta = \frac{E + E'}{k_BT}$$

Where E, and E′ represent the initial and final neutron energies, respectively.

$$\frac{d^2\sigma}{d\mu \, \mathrm{d}E'} = \sigma(E \to E', \mu) = \frac{\sigma_b}{2k_BT}\sqrt{\frac{E'}{E}}\, S(\alpha, \beta)$$

S(α,β) is the asymmetric form for the scattering law:

$$\mathrm{S}(\alpha, \beta) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} E^{i\beta\hat{t}} E^{-\gamma(\hat{t})} d\hat{t}$$

Where $\hat{t}$ the time expressed in units of $\hbar/(kT)$ and $\gamma(\hat{t})$:

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

$\rho(\beta)$ is the frequency spectrum of excitations of the scattering system (i.e., phonon density of states in a crystal), A is the atomic weight, k_B is Boltzman's constant, and T is the temperature.

Materials and methods

The forces and dynamical matrix of the lattice vibrations of the Bi were computed using the calculator Qauntum-expresso [3], [4] package. Bismuth has a rhombohedral structure with two atoms per unit cell. The rhombohedral angle is 57.23° and the atomic positional parameter z is 0.23389 at 298K. The lattice constant a_H is 4.546 Å and c_H is 11.863 Å [5]. Sapphire has a rhombohedral unit cell belonging to the R3c space group with a = 5.128 Å and α =55.28° [6]. The phonon frequency of Al_2O_3 Figure 1 was calculate by PhonoPy [7] based of the force constant was get from Phonon database [8]

The results of the estimated phonon frequency (lattice dynamics) in a single crystal, using a DFT code (Quantum-expresso) from the initial atomic configuration, each atom in the lattice cell is displaced by a small quantity. The displaced atom then sustains a, so-called Hellmann-Feynman, restoring force to come back to the stable structure. The dynamical matrix is obtained from these forces, and its Eigen-values are the energies of the vibrational modes in the crystal.

This computational resource is provided by iFit [9], with the sqw_phonon Model, which itself makes use of the Atomic Simulation Environment (ASE) [10]. In addition, the PhonoPy package is used to compute force constants.

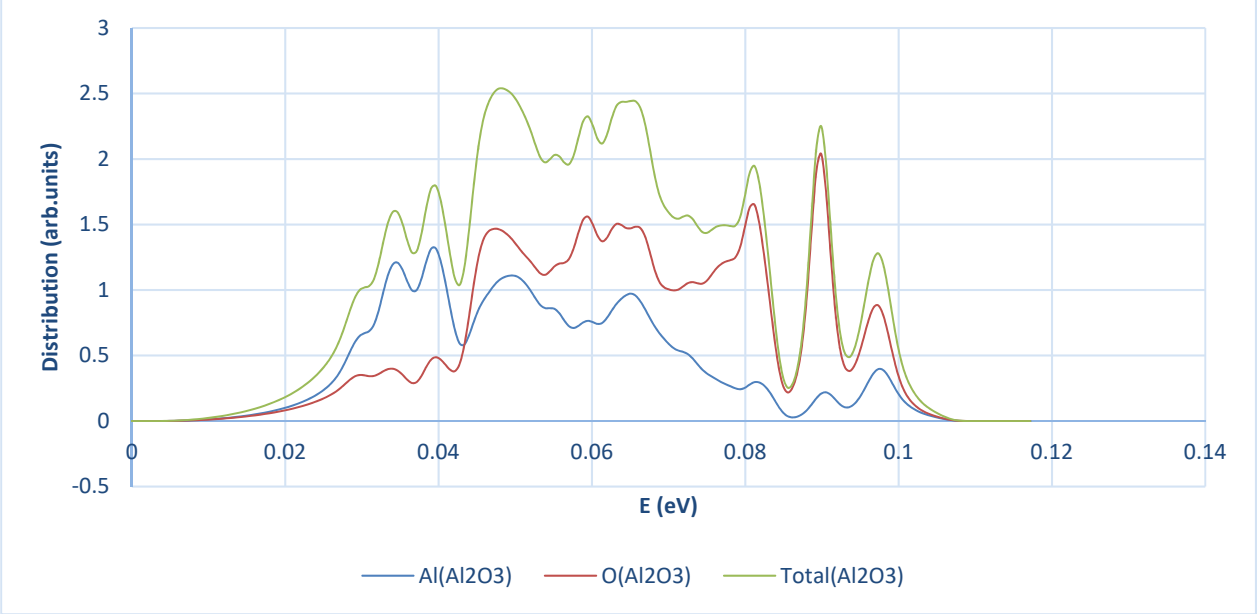

Figure 1: Phonon frequency of Al2O3

the vibrational density of states (aka phonon spectrum) for Bi is defined as the velocity auto-correlation function (VACF) of the particles are displayed in Figure 2.

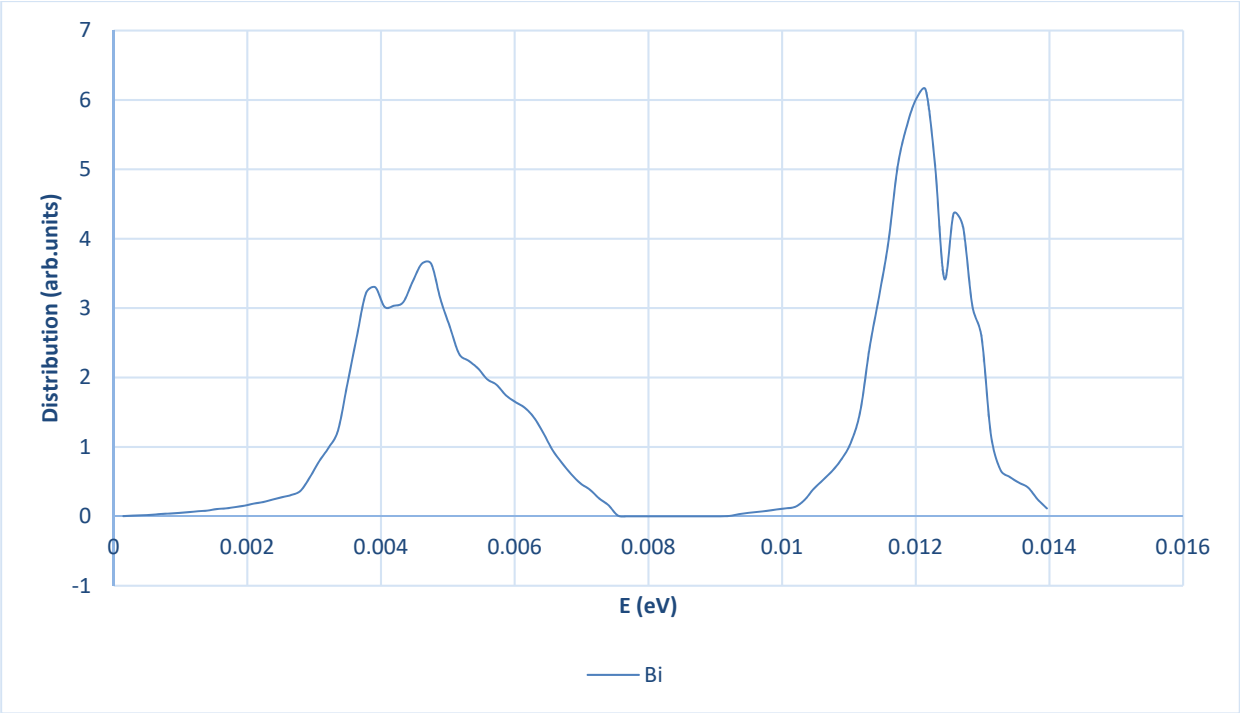

Figure 2: Phonon frequency of Bi

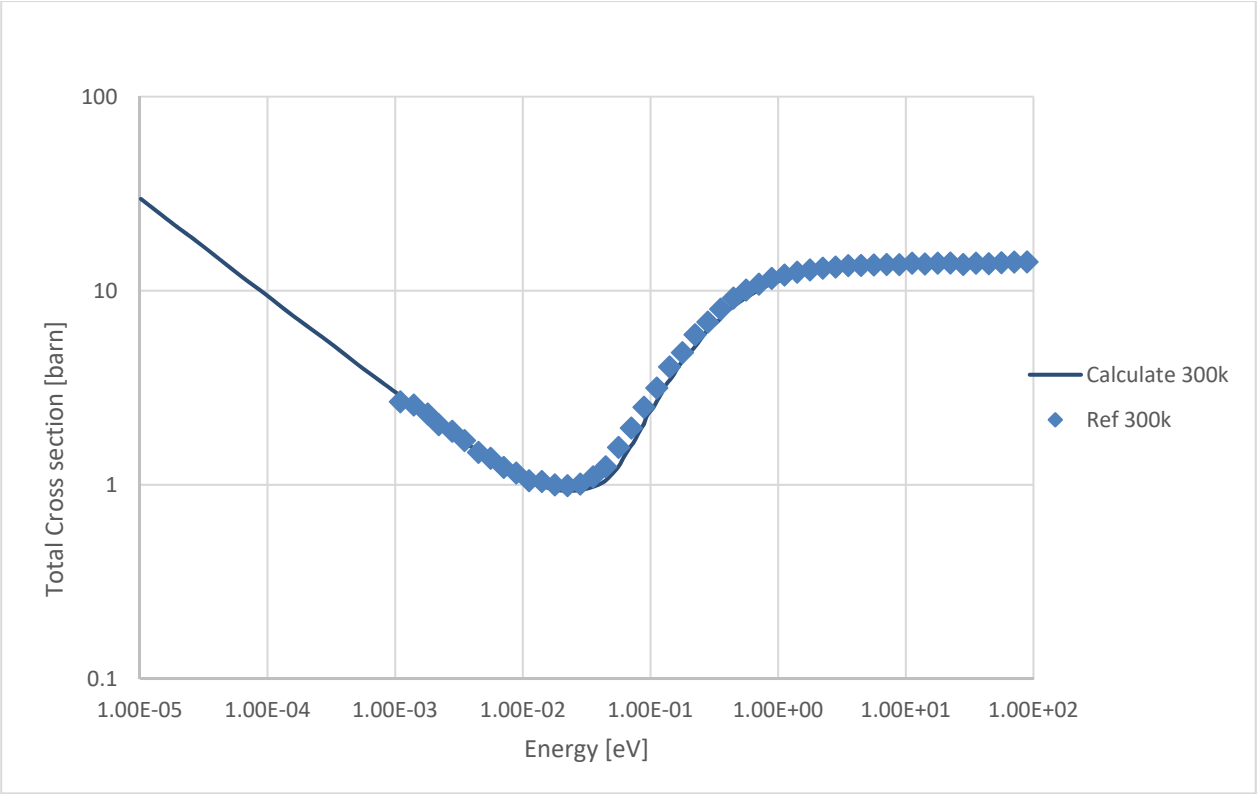

Figure 3: Comparison of the Total cross section for Al_2O_3

Results and discussion

Based on the data of the phonon frequency Figure1 and Figure2, the LEAPR module of the NJOY code was used to generate the Sapphire and the Bismuth thermal neutron scattering cross section at temperature 300 K for Sapphire and 80 K and 300 K for Bismuth.

For Sapphire crystal the thermal neutron scattering cross sections calculated by NJOY code are closer to experimental data [11].

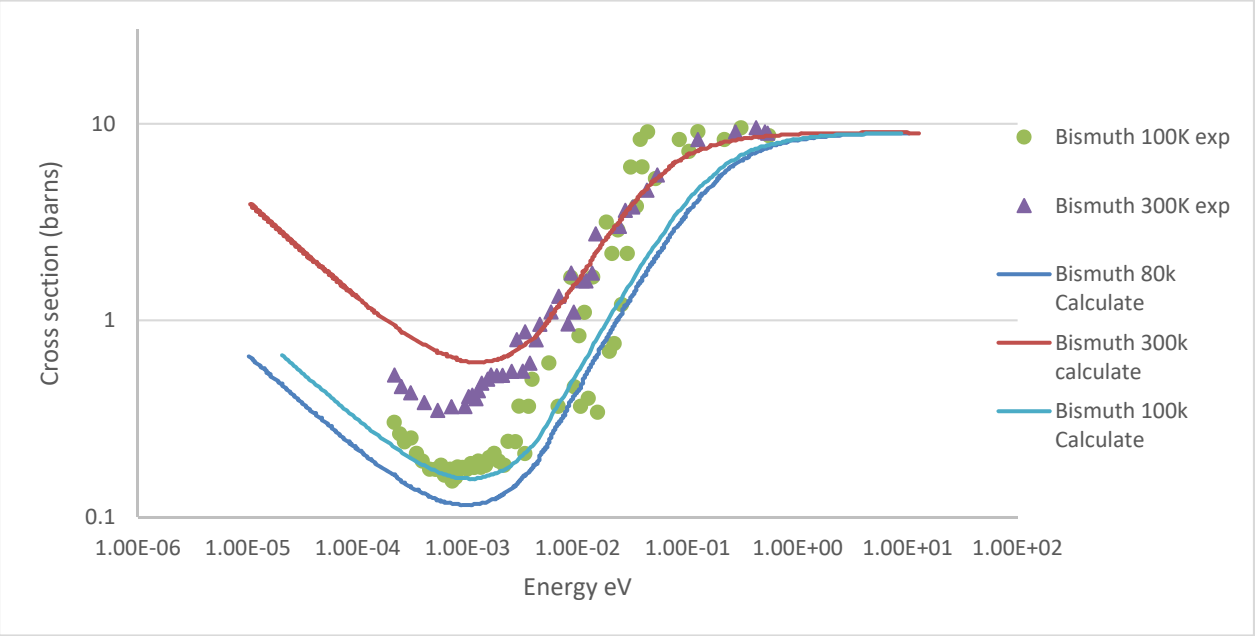

Figure 4: Comparison of the Total cross section for Bi

The Figure 4 show the comparison of total cross section of the Bismuth at room temperature and liquid nitrogen temperature. The calculated values using the NJOY v2016 code are acceptable with measured values. calculate [12]. For the difference of the cross section of the Bismuth crystal at room temperature in the range of energy below $2{,}51.10^{-3}$ eV due the calculation was performed for perfect crystal.

Conclusion

The computation of thermal neutron scattering for Sapphire and Bismuth single crystal was presented in this paper. The phonon frequency was determinate by Ifit, phonopy package and DFT code (Quantum-expresso). This frequency is implemented in LEAPR module of NJOY code to calculate thermal neutron scattering. The results were compared with the experimental data. The results were found to be in good agreement with the experimental data.

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