Study of Sapphire and MgO as Thermal Neutron Filters for the Moroccan TRIGA Research Reactor Beam

N. Zahar, D.Benchekroun, B.Belhorma, P.Hermet, C.Broeders

***Abstract*—In this contribution, the optimization of sapphire filter thickness was performed, for fast neutrons,with GEANT4. For thermal neutrons, interaction cross sections, based on the S(α,β) model, are not yet implemented in GEANT4. The present word focuses on the thermal neutrons interaction with $Al_2O_3$and MgO crystals, which are usually used are thermal neutron filters.The LEAPR module of NJOY code has been used to generate the thermal cross sections for $Al_2O_3$and MgO crystals, at different temperatures. The phonon density-of-state, required by the LEAPR module, has been calculated using the ABINIT package.The generated cross sections allowed us to study the temperature effect on the quality of each filter and to compare the filtering powers of the two considered crystals.**

***Keywords*— Reactor beam, Thermal neutron, Sapphire filter, Magnesium Oxide filter, temperature, GEANT4, S(α,β), LEAPR, NJOY.**

I. Introduction

THE single crystal sapphire Al_2O_3 is frequently used as fast neutron filter used in the experiments around the research reactors. The neutron filter material must have wavelength dependent cross section that is lower for thermal energies, less than 0.1 eV, and higher for energies greater than about 1 eV. The overall effect of the thermal neutron cross section σ_{th} is a superposition of several contributions: (a) absorption, σ_a ,normally proportional to neutron wavelength, (b) incoherent, σ_{inco}, (c) coherent inelastic , σ_{inel} and (d) any residual Bragg scattering, σ_{ela} which depends on neutron wavelength, crystal orientation and crystal perfection. Item (c) depends upon crystal temperature (phonon population), where coherent Bragg scattering can bedisallowed by using a special crystal orientation [1]:

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$$\sigma_{th} = \sigma_a + \sigma_{inco} + \sigma_{inel} + \sigma_{ela} \quad (1)$$

The effectiveness of such filter is given by the optimum filter thickness, crystal orientation and the temperature.One can also use the quality factor R, defined by the ratio of the total cross section at thermal energies, σ_{th}, to the total cross section at high energies, σ_{free}:

$$R = \frac{\sigma_{th}}{\sigma_{free}} \quad (2)$$

The absolute minimum value of R is obtained by neglecting σ_{ela} and σ_{inel} contributions:

$$R_{\min} = \frac{\sigma_a + \sigma_{inco}}{\sigma_{free}} \quad (3)$$

The lower value of R_{min} corresponds to the best filter. A low value for the numerator implies a good transmission of neutrons in the desired thermal energy range, while a large denominator ensures strong scattering of the unwanted epithermal and fast neutrons. The filter also acts to reduce the intensity of any γ-ray beam which accompanies the neutron beam.

II. Optimization of Sapphire Filter Thickness

The purpose of the present work is to find the optimal filter thickness that gives good fast neutronsattenuation and high transmission of thermal neutrons using GEANT4 code[2].The Monte Carlo code GEANT4 was used to calculate the transmission ratio of fast neutrons (E = 3 MeV) for different sapphire crystal thicknesses. Fig. 1 shows the fast neutrons transmission as a function of the crystal thickness L.

The calculated neutron transmission can be adjusted by the empirical function: $T = {}^{I}/_{I_0} = exp\left(-{}^{L}/_{\lambda}\right)$ (4)

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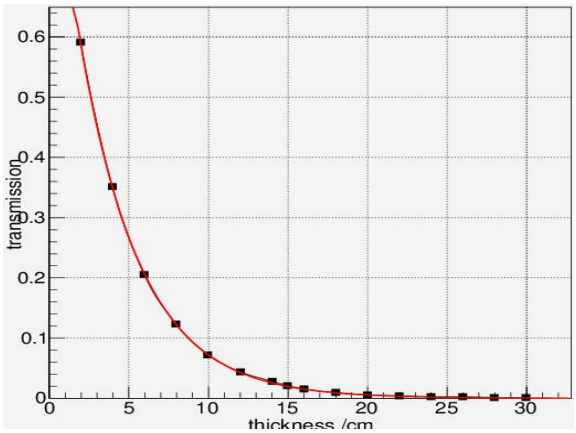

Fig. 1. Fast neutron transmission as a function of sapphire crystal thickness

The simulation results give a value of the λ parameter of 3.8 cm. For example, a sapphire thickness of 10 cm could absorb about 95% of fast neutrons. Similar results have been found by I.E. Stamatelatos and S. Messoloras [3].

However, for the same thickness, the calculated transmission rate of thermal neutrons is about 6.5%which does not suit the purpose of a thermal neutron filter.The reason of this disagreement comes from the thermal cross sections that are not correctly implemented in Geant4 for a lot of materials.

The Geant4 code can treat the physically reliable transport of thermal neutrons if the S(α,β), inelastic cross section data are used. In this case, it takesinto account atomic translational motion as well as vibration and rotation of the bound atoms that also significantly affect the cross sections and final states. The current G4NDL4.2.TS data librarycontains S(α,β) data for some molecules, such as H bounded in ZrH. However, there is no ENDF data library for Al_2O_3. The main task of the next steps is to generate thermal scattering data for the Al_2O_3 crystal (sapphire)and incorporate it in the GEANT4 database.

III. Thermal Neutron Scattering Cross Section

The calculating of thermal neutron scattering cross sections in such material would include information on the absorption and inelastic scattering since the elastic scattering is neglected. The inelastic scattering cross sections are calculated by using NJOY code [4]. The phonon frequency distribution, generated independently by ab-initio calculations, is the main input for accurate thermal cross sections determination at various temperatures.

A. Phonon Frequency Generation for Al_2O_3 and MgO :

Born effective charge tensor and dynamicalmatrices of Al_2O_3 and MgO were computed within a variational approach to density functional perturbation theory as implemented in the ABINIT package [5]. The exchange-correlation energy functional was evaluated within the generalized gradient approximation according to Perdew, Burke and Ernzerhof scheme [6]. Al($3s^2$, $3p^1$), Mg($3s^2$) and O($2s^2$, $2p^4$)-electrons were considered as valence states in the construction of the pseudopotentials. The electronic wavefunctions were expanded in plane-waves up to a kinetic energy cutoff of 57 Ha. Integrals over the Brillouin zone were approximated by sums over a 8*8*8 mesh of special k-points [7]. Atomic positions of each structure were relaxed at their corresponding experimental volume and lattice parameters: rhombohedralunit cell belonging to the $R\bar{3}c$ space groupwith a =5.128 $\mathring{A}$ andα =55.28° for Al_2O_3 [8], and cubic unit cell belonging to the $Fm\bar{3}m$ space group with a =2.979 $\mathring{A}$ and α =60° for MgO [9]. Phonon dispersion curves were interpolated according to the scheme described in ref [10]. In this scheme, the long-range character of the dipole-dipole contribution is correctly handled by first subtracting it from the force constant matrix in reciprocal space and treating it separately. The short-range contribution to the interatomic force constants in real space is then obtained from the remainder of the force constant matrix in q-space using a discrete Fourier transform. From the resulting set of interatomic force constants in real space, phonons can be readily obtained at any point in the Brillouin zone. For the both materials, a 150 * 150 * 150 q-points grid in the irreducible Brillouin zone was employed for the calculation of the integrals associated to the phonon density -of-states. They are displayed at 0 K in Figs. 2 and 3 respectively for Al_2O_3 and MgO

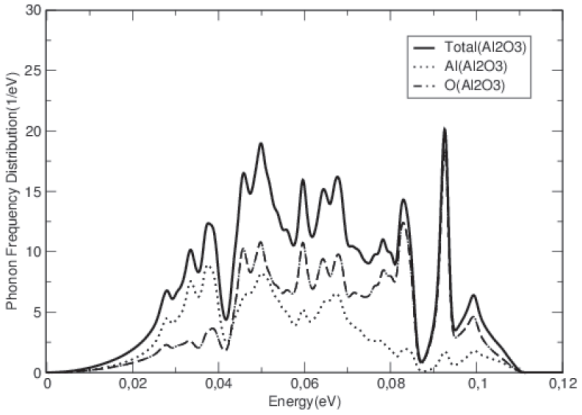

Fig. 2. Partial and total phonon frequency distributions for Al_2O_3

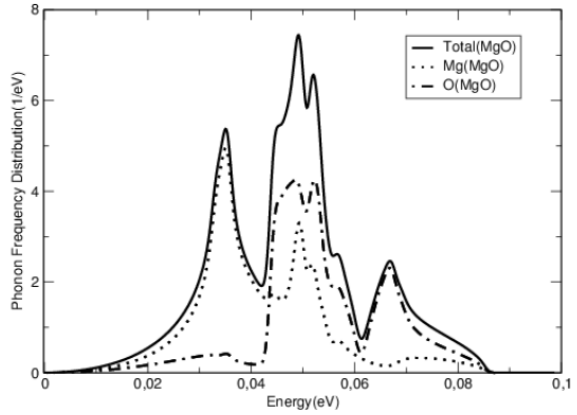

Fig. 3.Partial and total phonon frequency distribution for MgO

B. Thermal Inelastic Cross Section

The calculation of inelastic cross section,based on the S(α,β) model, for sapphire crystal,was handled by LEAPR module of the NJOY tool. Fig. 4 shows the total neutron cross section per Al_2O_3 molecule at room temperature (300 K).

The results are in a good agreement with experimental data and show a minimum around the thermal energy which could ensure a good transmission of thermal neutrons. For higher energies, the cross sections are compatible with those derived from the free-atom assumption.

In Fig. 5 are compared the total neutron cross section in sapphire at room and liquid nitrogen temperatures (300 K and 77 K). One can see that the filter quality is considerably improved by cooling the crystal. The real effect of the temperature on the filter quality will be discussed in the next section. The same work has been performed for the magnesium oxide crystal (Figs 6 and 7).

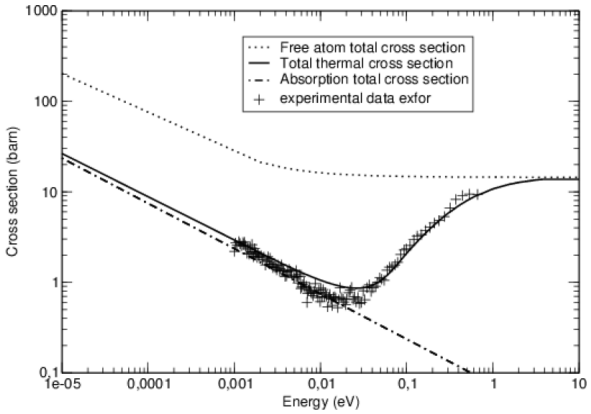

Fig. 4. Total cross section per molecule for sapphire crystal at 300 K

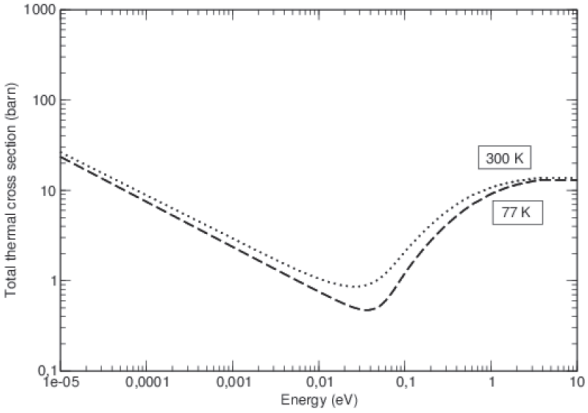

Fig. 5. Total thermal cross section per molecule for sapphire crystal at300 K and 77 K

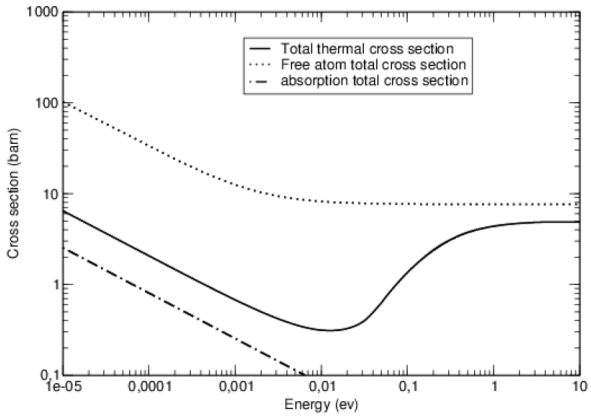

Fig. 6. Total cross section per molecule for magnesium oxide crystal at 300 K

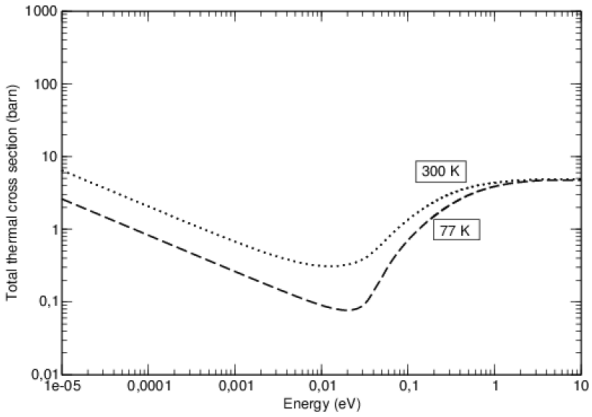

Fig. 7. Total thermal cross section per molecule for magnesium oxide crystal at 300 K and 77 K

IV. Remarks and Discussion

To show the effect of cooled filter sapphire Al_2O_3 and magnesium Oxide MgO at liquid nitrogen and room temperature to attenuate fast, epithermal neutron and transmission of thermal neutron, the quality factor were calculated. Tables I and II list respectively $R_{\min}$ for sapphire and magnesium oxide filter materials, at both temperatures.

At both temperatures, the MgO filter seems to have a slightly better quality than sapphire filter. Also, the improvement of the quality factor by the crystal cooling is higher for MgO than for Al_2O_3.

If we assume that the transmission rate is given by

$$T_n = \frac{I_x}{I_0} = e^{-n\sigma_{th}x}$$

σ_{th} = total cross section calculated by the NJOY code,
n = number of molecules per volume unit and
x = crystal thickness.

The estimated value of the thermal transmission rate ($E \approx 0.025$ eV)at room temperature, for a 10 cm thick sapphire crystal, is about 81.7 % which is in agreement with the results of R. Born at al. [11] and N. Habib [1].

The thermal transmission rate at liquid nitrogen temperature (77 K) can be calculated as before by using the thermal cross section at T = 77 K. The comparison of the two transmission rates show that only a small increase ≈ 8% is achieved by cooling the crystal at 77 K. Such a small increase could be insufficient to warrant the expense of cryogenics.

For MgO crystal, the transmission rate at 300 K is about 77.4%, which is less efficient than sapphire crystal. But cooling the MgO crystal at 77 K improves the thermal transmission by a factor 24%. The crystal cooling is well justified in the case of MgO filter. The conclusions have been done by D.F.R. Mildner et al. [12].

TABLE I
QUALITY FACTOR FOR AL_2O_3

Al_2O_3		
Energy(eV)	R_{min} [300 K]	R_{min} [77 K]
0.014	0.06003	0.0408
0.024	0.0563	0.0335
1.0018	0.7397	0.6283
3.0014	0.92665	0.8691

TABLE II
QUALITY FACTOR FOR MGO

MgO		
Energy(eV)	R_{min} [300 K]	R_{min} [77 K]
0.014	0.0515	0.025
0.024	0.046	0.0205
1.0018	0.5741	0.5101
3.0014	0.6329	0.6106

V. CONCLUSION

The thermal neutron cross sections have been generated by the NJOY code, to estimate the transmission of thermal and fast neutrons through sapphire and MgO crystals. The cross sections generation is based on the S(α,β) model is a long procedure beginning from ab-initio calculation of phonon spectrum and leading to a cross section distribution to be validated by experimental data. The obtained cross sections can be used to estimate the quality of each filter at different temperatures.

The results show that, at room temperature, sapphire filter has a slightly better thermal transmission rate than MgO filter. The cooling of the crystal at liquid nitrogen temperature improves significantly the filtering quality of the MgO filter while the gain for sapphire does not justify the cost of cooling.

The generated cross sections are being translated to the G4NDL format, to be implemented in Geant4. This step is performed with the help of the Geant4 collaboration, thanks to Tatsumi KOI.

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