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POLYCRYSTALLINE BERYLLIUM AND GRAPHITE AS COLD NEUTRON FILTERS

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The total neutron cross-section of polycrystalline beryllium and graphite has been calculated beyond the cut-off wavelength using a general formula. The computer COLDFILTER code was developed in order to provide the required calculations. The calculated neutron transmissions through polycrystalline Be and graphite at different temperatures were compared with the experimental data measured at the ET-RR-1 reactor using two TOF spectrometers. An overall agreement is obtained between the formula fits and experimental data at different temperatures. A feasibility study is carried on using polycrystalline Be as an efficient filter for neutrons with energies less than 5 meV ($\lambda > 0.4$ nm), while graphite for energies less than 1.8 meV. Calculations show that the 20 cm polycrystalline Be cooled to the Liquid Nitrogen (LN_2) temperature transmits more than 85% of incident neutrons with energies less than 5 meV and rejects ($T_n < 1\%$) neutrons with higher energies. While the 10 cm thick polycrystalline graphite cooled to the LN_2 temperature has a higher effect–to-noise ratio than that for Be for incident neutron energies less than 1.8 meV.

Keywords: *Cold neutron filters; polycrystalline Be and Graphite.*

INTRODUCTION

Neutron diffraction powder investigation is usually carried out with wavelengths ranging from 0.10 to 0.15 nm. Although longer wavelengths can lead to an increased resolution, their use is limited due to higher-order contamination problems. The development of the triple-axis spectrometer for inelastic neutron scattering has proved invaluable for excitations in solids, liquids, and gases [1]. This spectrometer requires a monochromator to select single incident neutron energy and an analyzer to determine the energy of neutrons scattered from a sample. In some cases, the spectrometers are required to operate in gain energy mode [2]. Such a mode simplifies the analysis of measured phonon spectrum. When using such mode the selected neutrons are of wavelengths longer than 0.4 nm (cold neutrons) [3].

It is well known that, the coherent elastic scattering by a crystalline material cannot occur for neutrons with wavelengths which exceed some maximum value of λ_{max}, where λ_{max} is given by $\lambda_{max} = 2d_{max}$, and d_{max} is the largest d spacing of planes in the crystal. The variation of the scattering cross-section in the vicinity of λ_{max} for a number of polycrystalline filters, of which Be, BeO, and graphite are perhaps the most commonly used [4]. The inelastic contribution may be reduced by cooling the material to liquid nitrogen temperature.

A sufficiently thick filter will then transmit a beam of cold neutrons with little attenuation, while reducing the intensity with $\lambda \prec \lambda_{max}$ by three or four orders of magnitude.

It was shown by Freund [5] that the total cross-section determining the attenuation of neutrons by a crystalline material can be given by a semi-empirical formula. In this formula Freund [5] neglected the contribution of the Bragg scattering due to reflections from crystal planes of the total attenuation of neutrons. Naguib and Adib [6,7] reported a formula which allows to calculate the contribution of the Bragg scattering from different (hkl) planes to the neutron on transmission through crystalline material.

The present work concerns a feasibility study for use of Be and graphite as a cold neutron filter. The optimum Be and graphite thickness and their temperature for efficiently transmitting the cold reactor neutrons while rejecting both fast neutrons and gamma rays accompanying the cold ones are also given.

THEORETICAL TREATMENT

The total cross-section determining the attenuation of neutrons by a crystalline solid is given by

$$\sigma = \sigma_{abs} + \sigma_{tds} + \sigma_{Bragg} \qquad (1)$$

where the neutron capture cross-section (i.e. absorption) σ_{abs} for Be and graphite obeys the $1/\sqrt{E}$ law, and can be written as : $\sigma_{abs} = C_1 E^{-1/2}$, where E the neutron energy and C_1 a constant which can be calculated from values provided by Sears [8].

As shown by Freund [5], the second contribution σ_{tds} can be split in two parts, σ_{mph} (multiple phonon) and σ_{sph} (single phonon), depending on neutron energy

$$\sigma_{tds} = \left[A/(A+1)\right]^2 \sigma_{bat}\left[1-e^{-WC_2E}\right] + E^{-1/2}\left[C_1 + \frac{\theta_D^{1/2}\sigma_{bat}}{36A}\begin{cases} R \ldots\ldots\ldots\ldots\ldots X \le 6 \\ 3.3X^{-7/2} \ldots X > 6 \end{cases}\right] \quad (2)$$

where e^{-W} is the Debye-Waller factor [9], C_2 is a constant which is dependent on the scattering material and given by $C_2 = 4.27\exp[A/61]$, Freund [9] , $X = \theta_D / T$ (T is the sample temperature), σ_{bat} is the sum of coherent and incoherent scattering cross-sections of the bound atom), A in case of compounds is the average atomic mass number, and the series R is given by $R = \sum_{n=0}^{22} B_n X^{n-1} \big/ \left[n!(n+5/2)\right]$, with B_n being the Bernoulli numbers.

The single phonon scattering cross-section concerns the energy range $E << k_B\theta_D$, where k_B is Boltzmann's constant and θ_D is the Debye temperature characteristic of a material. It is determined by phonon annihilation processes. Second part of TDS is predominant in the range $E \ge k_B T$, where also down scattering and multi-phonon processes occur.

However, using the static incoherent approximation, Cassels [9] has estimated the short-wavelength elastic cross-section, which is extinct for perfect single crystals. Hence the multi-phonon scattering cross-section in the range $E >> k_B\theta$, given by the first term of Eq.(2), can be replaced by:

$$\sigma_{mph} = \sigma_{free}\left\{1-\left(\lambda^2/2W\right)\left[1-\exp\left(-2W/\lambda^2\right)\right]\right\} \quad (3)$$

The contribution of Bragg scattering σ_{Bragg} to the total cross section taking into account the resulting reflection from different (*hkl*) planes, which are able of giving the Bragg reflection for the neutron wavelength λ, was calculated. In case of poly-crystalline material, the reflections are from all planes having spacing $d_{hkl} \ge \lambda/2$.

It was shown by Bacon [10] that for a polycrystalline material with grain size less than 10^{-4} mm, the total coherent Bragg scattering cross-section can be given as:

$$\sigma_{Bragg} = \frac{N_c\lambda^2}{2}\sum_{d_{hkl} \ge \lambda/2} F_{hkl}^2\, d_{hkl}\,.e^{-2w} \quad (4)$$

where N_c is the number of unit cells per cubic centimeter , F_{hkl} is the structure factor of the unit cell and e^{-2w} is the Debye-Waller factor.

A computer code COLDFILTER is an adapted version of ISCANF and ISCANF-II codes developed in order to provide the required calculations [6,7]. The code is based on the calculation of nuclear absorption σ_{abs} and the thermal diffuse scattering cross-section σ_{tds} contribution for long-wavelength in similar way as given ISCANFII [7] while for short- wavelength using the static incoherent approximation [9]. The code also includes the calculation of the Bragg scattering term given by Equation (4).

For comparison of the experimental transmission data with the calculated values, the code takes into consideration the effects of both neutron wavelength resolution and incident neutron beam divergence [10].

COMPARISON WITH EXPERIMENT

In order to check the applicability of the deduced formula, the calculations were carried out for polycrystalline Be and graphite and compared with the experimental ones. The main Be and graphite physical parameters used for the calculations are listed in Table 1.

Table 1. Physical parameters of Be and graphite.

Physical parameter	Be	Graphite
Atomic Weight	9.0	12
Crystal Structure	HCP	HCP
Lattice Constants	a = 0.2275 nm	a = b = 0.2464 nm,
	c = 0.358 nm	c = 0.6736 nm
Number of atoms/ unit cell	2	4
Atomic Positions	1/3 2/3 1/4, 2/3 1/3 3/4	0,0,0 ; 0,0,½; ⅔,⅓,0 ; ⅓,⅔,½
Number of unit cells/cm^3	0.6165 E +29	2.89 E+28
Debye Temperature	1100 K	1050 K
Neutron capture cross-section	1.68 mb	0.0031 b
at 0.025 eV	7.631 b	5.555 b
σ_{bat}	7.746 fm	
Coherent Scattering amplitude		6.61 fm

Polycrystalline Be

The neutron transmission through 4 cm Be at the room temperature was calculated in the energy range from 2 meV up to 2 eV (wavelength band from 0.2 nm - 0.6 nm) using the COLDFILTER code. The result of calculations is displayed in Figure 1 by solid line. For comparison the available experimental values, measured for the 4 cm polycrystalline Be at the room temperature [11], were also displayed in Figure 1 by dots.

From the figure one can notice that, the calculated values at the room temperature are in a reasonable agreement with the experimental ones.

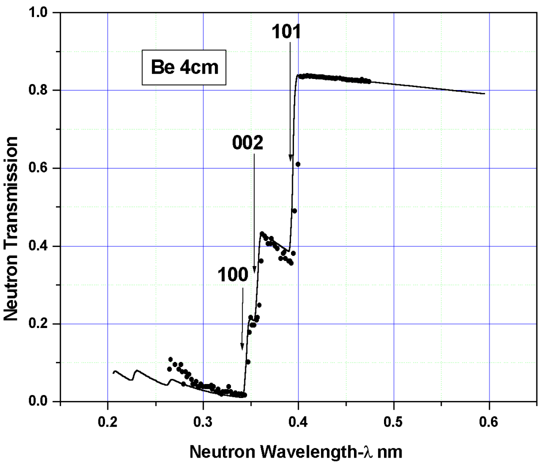

Figure 1. Neutron transmission through 4 cm polycrystalline Be.

To show the effect of both thickness and temperature of the polycrystalline Be on its filtering characteristics, the calculations were performed at room and liquid nitrogen temperatures in the energy range from 2 meV up to 2 eV. The results of these calculations are displayed in Figure 2.

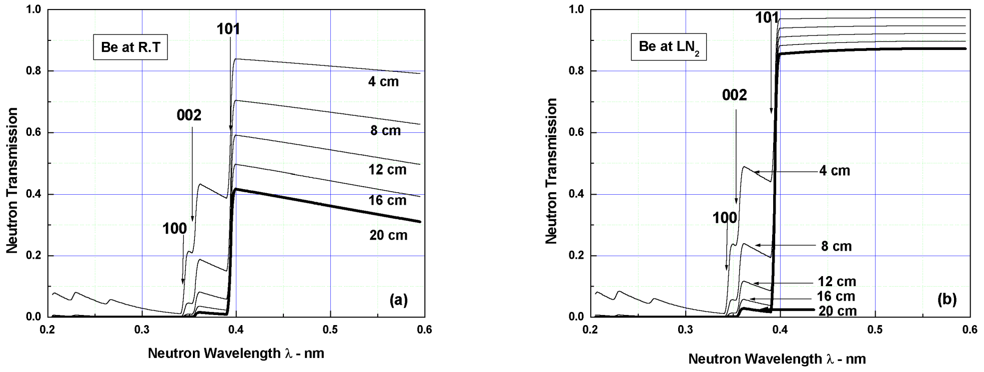

Figure 2. Calculated neutron transmissions through polycrystalline beryllium

The neutron flux having Maxwellian distribution with neutron gas temperature close to room temperature (300 K) transmitted through the 20 cm thick polycrystalline

Be at room and liquid nitrogen temperatures are displayed in Figure 3a. Figure 3b shows the transmitted neutron flux with neutron gas temperature close to liquid hydrogen one.

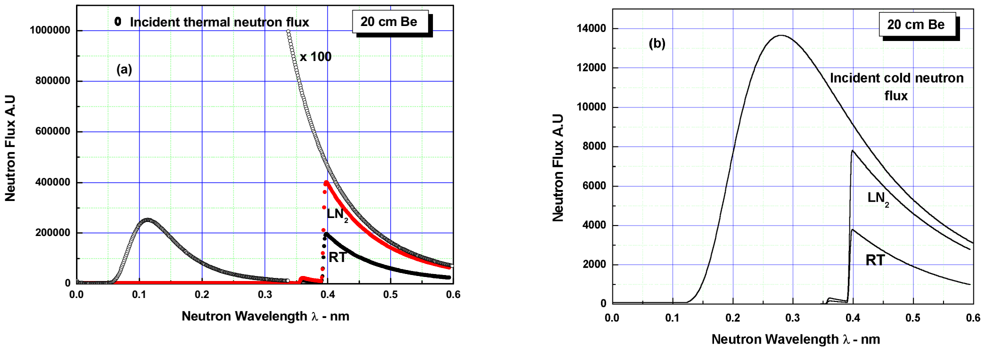

Figure 3. Transmitted neutron flux through polycrystalline beryllium

It is apparent that Be can be efficiently used as a cold neutron filter specially for neutrons emitted from cold neutron source. The 20 cm polycrystalline Be cooled to the LN_2 temperature transmits more than 85% of incident neutrons with energies less than 5 meV while rejects ($T_n < 1$ %) neutrons with higher energies.

Polycrystalline graphite

The total cross-sections of graphite at temperatures of 300 K and 478 K were calculated for neutrons in the energy range from 0.1meV up to 1 eV. The results of these calculations are displayed in Figure 4 by solid lines. For comparison, the experimental data [12] measured at the ET_RR-1 are also displayed in Figure 4.The calculated data are almost in agreement with experimental values for the fitted parameters C_2=5.0 and θ_D=1050 K. One can observe that the graphite total cross-section beyond the cut-off wavelength $\lambda_c=2d_{oo2}$ (at E< 1.8 meV) is about 0.6 barn. This value is much less than the free atomic cross-section 4.7 barns at neutron energies higher than 1 eV.

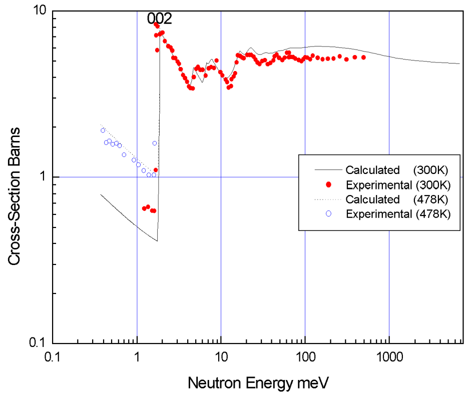

Figure 4. The total neutron cross-section of polycrystalline graphite

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To show the effect of both thickness and temperature of polycrystalline graphite on its filtering features, the calculations were performed at room and LN$_2$ temperatures, for neutrons in the energy range 10^{-3} – 1 eV. The results of these calculations are displayed in Figure 5. The indication is that the 10cm thick polycrystalline graphite cooled to the LN$_2$ temperature, has a better effect-to-noise ratio for neutrons with

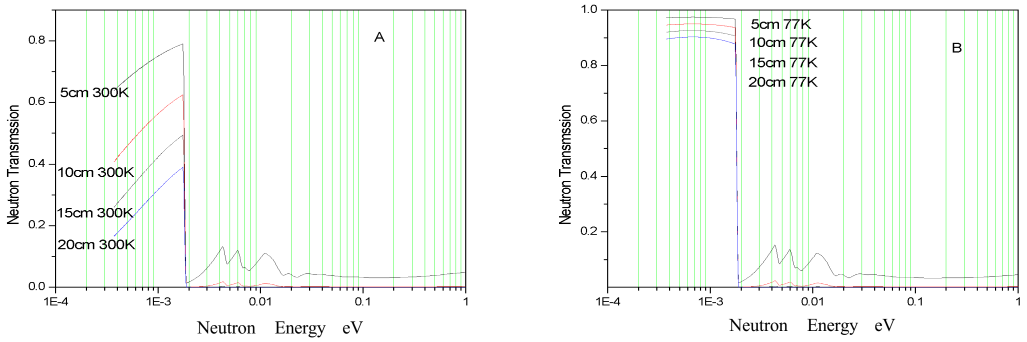

Figure 5. Neutron transmission through polycrystalline graphite

The calculation of the cold neutron flux, for which there is a Maxwellian distribution with a neutron gas temperature close to the liquid hydrogen one, is displayed in Figure 6 before and after its transmission through the 10 cm thick polycrystalline graphite cooled to 77 K. It is observed that the 10cm graphite transmits about 90 % neutrons with wavelength ≥ 0.67 nm. One can conclude that polycrystalline graphite under these conditions provides a high intensity of transmitted cold neutrons, while efficiently removes the epithermal and fast neutrons (less than 0.1 %).

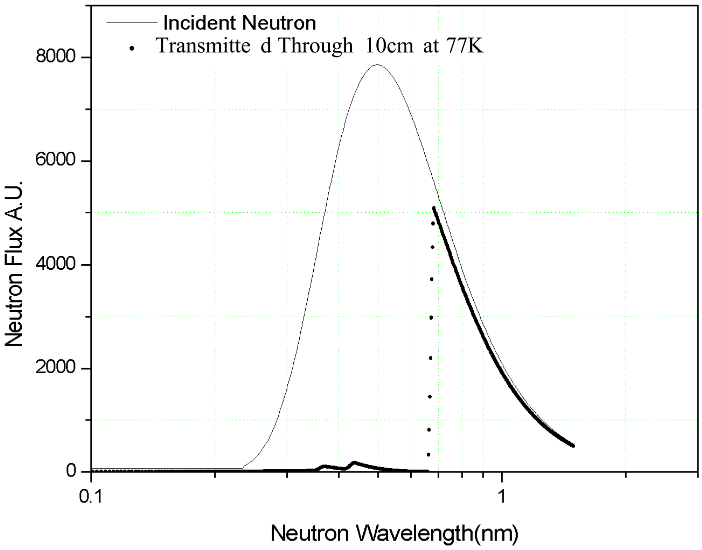

Figure 6. Transmitted cold neutron flux through polycrystalline graphite

CONCLUSION

The developed COLDFILTER code based on a general formula permits to calculate, the total cross-section of polycrystalline beryllium and graphite, within accuracy sufficient for determining its filtering characteristic s.

Calculations show that the 20 cm polycrystalline Be cooled to the LN_2 temperature transmits more than 85% of incident neutr ons with energies less than 5 meV while rejects ($T_n < 1$ %) neutrons with higher energies.

Calculations show that, the 10 cm thick polycrystalline graphite cooled to the LN_2 temperature has a higher effect to- noise- ratio than that for Be for incident neutron energies less than 1.8 meV.

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عديد بلورات البريليوم والجرافيت كمرشح للنيوترونات الباردة

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تم استخدام معادلة عامة لحساب المقطع المستعرض الكلى للنيوترونات ذات الطول الموجى خلف القطع النيوترونى للبريليوم والجرافيت عديد البلورات.

وقد تم تصميم واستخدام برنامج COLDFILTER لاجراء الحسابات. وقد تمت مقارنة قيم النفاذية النيوترونية للبريليوم والجرافيت عند درجات حرارة مختلفه مع القيم المعملية المقاسة على مفاعل الابحاث المصرى الأول باستخدام مطيافى زمن الطيران. هذا وقد تم الحصول على اتفاق عام بين القيم المحسوبة من المعادلة والقيم العملية لدرجات الحرارة المختلفة.

وقد أجربت دراسة جدوى لاستخدام البريليوم عديد البلورات كمرشح فعال للنيوترونات وأظهرت الحسابات أن سمك ٢٠ سم من البريليوم مبرد إلى درجة حرارة النيتروجين السائل يسمح بمرور ٨٥ % للنيوترونات الساقطة بطاقات أقل من ٥ مللىالكترون فولت بينما يمرر أقل من ١% من النيوترونات ذات الطاقات الأعلى. فى حين أن سمك ١٠ سم من الجرافيت المبرد عند درجة حرارة النيتروجين السائل له كفاءة أعلى من البريليوم لطاقات النيوترونات أقل من ١,٨ مللى الكترون فولت٠