POLYCRYSTALLINE MATERIALS AS A COLD NEUTRON AND GAMMA RADIATION FILTER.

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The total neutron cross-section of polycrystalline beryllium, graphite and iron has been calculated beyond their cut-off wavelength using a general formula. The computer COLDFILTER code was developed in order to provide the required calculations. The code also permits the calculation of attenuation of reactor gamma radiation,

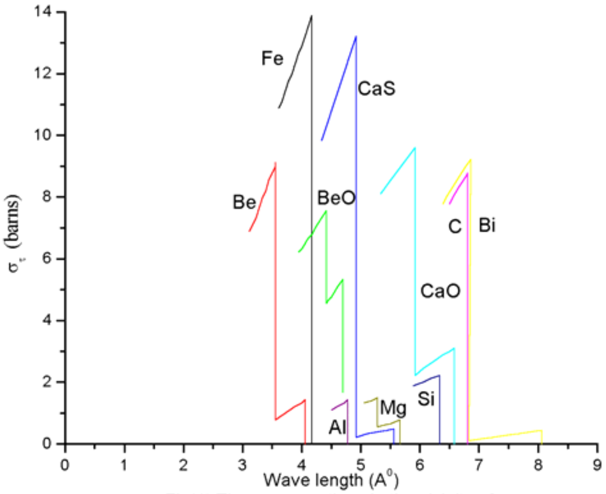
The calculated neutron transmissions through polycrystalline Be graphite and iron at different temperatures were compared with the experimental data measured at the ET-RR-1 reactor using two TOF spectrometers. An overall agreement is obtained between the formula fits and experimental data at different temperatures.

A feasibility study is carried on using polycrystalline Be, graphite and iron an efficient filter for cold neutrons and gamma radiation.

INTRODUCTION

Gamma radiation, fast and thermal neutrons are all associated with fission reactors. The thermal neutrons are a powerful tool for investigation of the structure and dynamic of solid state and liquids. To improve the effect to noise ratio, the development of thermal neutron filters is required.

As shown by several authors [1-4], poly- and mono- crystals nowadays are commonly used as thermal neutron filter. The coherent elastic scattering by a crystalline material can not occur for neutrons with wavelength λ_{max} which exceed twice the largest d-spacing of the possible reflections. In case of a powdered sample (poly-crystalline material) there is a steep increase of the coherent elastic scattering cross-section. Fig(1) shows the variation of scattering cross-section of which Fe, Be, BeO and graphite are perhaps the most suitable materials when used as a cold neutron filter.



Fig(1) The cross sections in the vicinity of the Bragg cut-off wavelengths for a number of poly-crystalline materials

However the best filter materials will be those for which the remaining contribution to the cross-section are also small for $\lambda > \lambda_{max}$. Therefore it is worthwhile to carry out a feasibility study of using poly-crystalline Fe as a cold neutron filter. In case of a single crystal the coherent scattering is characterized by discrete spectrum of peaks whose heights may exceed the value of coherent scattering cross-section of a powder. The peak heights and width of the spectra are found to depend on the crystal structure type, its mosaic spread value, the plane along which the crystal surface is cut and its orientation with respect to neutron beam direction.

The present work concerns a feasibility study for use of Be, graphite and iron as a cold neutron filter. The optimum Be, graphite and iron 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

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

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 [5].

As shown by Freund [6], the second contribution σ_{tds} can be split in two parts, σ_{mph} (multiple phonon) and σ_{sph} (single phonon), depending on neutron energy

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

where e^{-W} is the Debye-Waller factor [7], C_2 is a constant which is dependent on the scattering material and given by $C_2 = 4.27\exp[A/61]$, Freund [6] , $X = \theta_D/T$ (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 $R = \sum_{n=0}^{22} B_n X^{n-1} / [n!(n+5/2)]$, 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≥ $k_B T$, where also down scattering and multi-phonon processes occur.

However, using the static incoherent approximation, Cassels [8] 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:

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

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 $d_{hkl} \geq \lambda/2$

It was shown by Bacon [7] that for a polycrystalline material with grain size less than 10^{-4} mm, the total coherent Bragg scattering cross-section can be given as:

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

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 COLDFILTER code is an adapted version of ISCANF and ISCANF-II codes developed in order to provide the required calculations [9, 10]. 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 [10] 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 [11].

Comparison with Experiment

In order to check the applicability of the deduced formula, the calculations were carried out for poly-crystalline Be, graphite and iron and compared with the experimental ones. The main Be, graphite and iron physical parameters used for the calculations are listed in Table1.

Table 1. Physical parameters of Be , graphite and iron.

Physical parameter	Be	Graphite	Iron
Atomic Weight	9.0	12	55.85
Crystal Structure	HCP	HCP	BCC
Lattice Constants	a = 0.2275 nm c = 0.358 nm	a = b = 0.2464 nm, c = 0.6736 nm	a_o = 0.286 nm
Number of atoms/ unit cell	2	4	2
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	0,0,0;0.5,0.5,0.5
Number of unit cells/cm^3	0.6165 E +29	2.89 E+28	4.28 E+28
Debye Temperature	1100 K	1050 K	900 K
Neutron capture cross-section at 0.025 eV	1.68 mb	0.0031 b	2.56 barns
σ_{bat}	7.631 b	5.555 b	8.606 b
Coherent Scattering amplitude	7.746 fm	6.61 fm	9.4 fm

1. 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 Fig.(2) by solid line. For comparison the available experimental values, measured for the 4 cm polycrystalline Be at the room temperature [12], were also displayed in Fig.(2) 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.

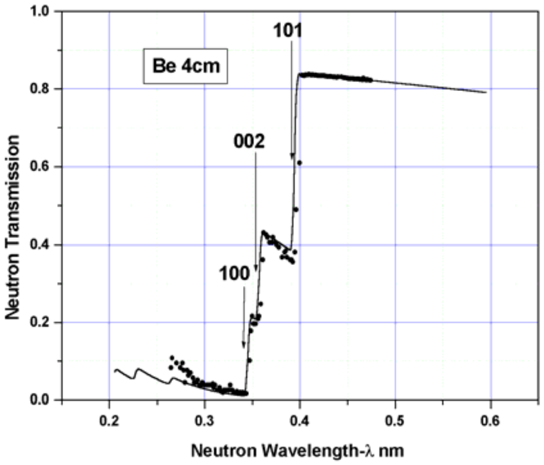


Fig. (2). Neutron transmission through 4 cm polycrystalline Be

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 Fig.(3).

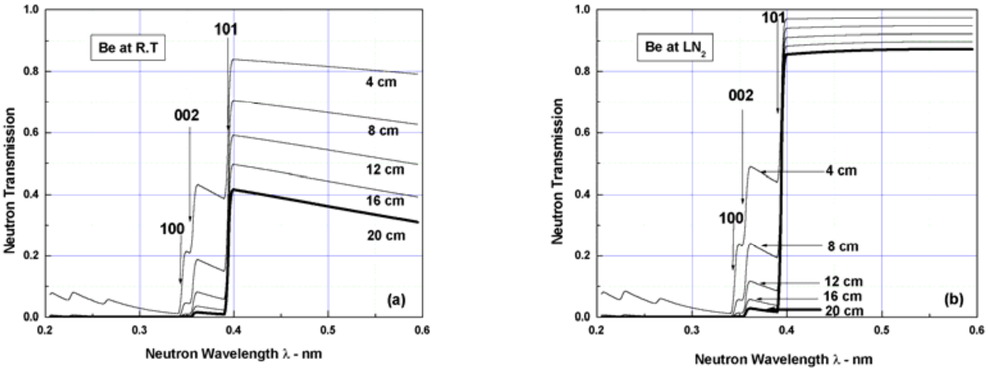


Fig. (3). Calculated neutron transmissions through polycrystalline beryllium

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 Fig. (4)a. Fig.(4)b shows the transmitted neutron flux with neutron gas temperature close to liquid hydrogen one.

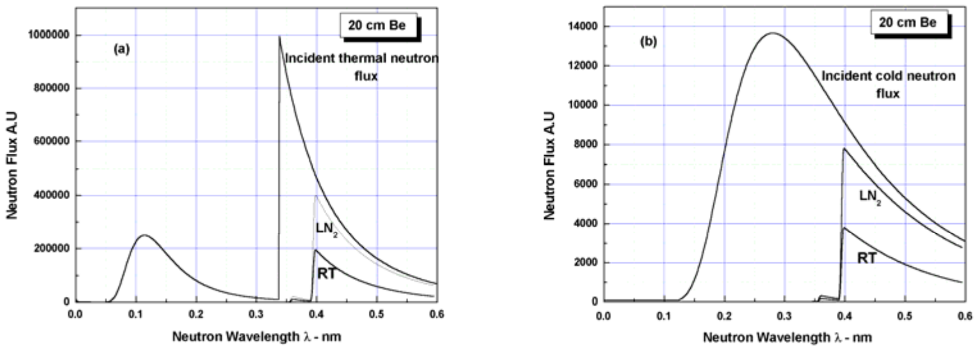


Fig. (4). Transmitted neutron flux through polycrystalline beryllium

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.

2. 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 1eV. The results of these calculations are displayed in Fig. (5) by solid lines. For comparison, the experimental data [13] measured at the ET_RR-1 are also displayed in Figure 5.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< 1.8meV) is about 0.6 barn. This value is much less than the free atomic cross-section 4.7 barns at neutron energies higher than 1eV..

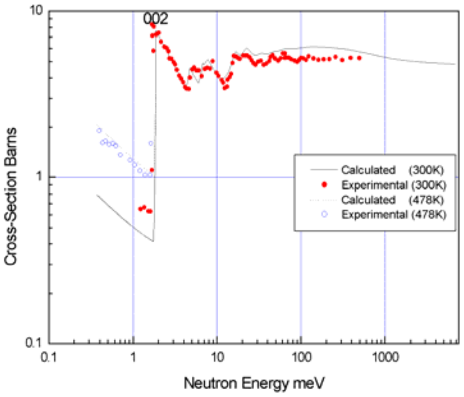


Fig. (5). The total neutron cross-section of polycrystalline graphite

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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} – 1eV. The results of these calculations are displayed in Figure6. The indication is that the 10 cm thick polycrystalline graphite cooled to the LN_2 temperature, has a better effect-to-noise ratio for neutrons with wavelengths ≥ 0.671nm.

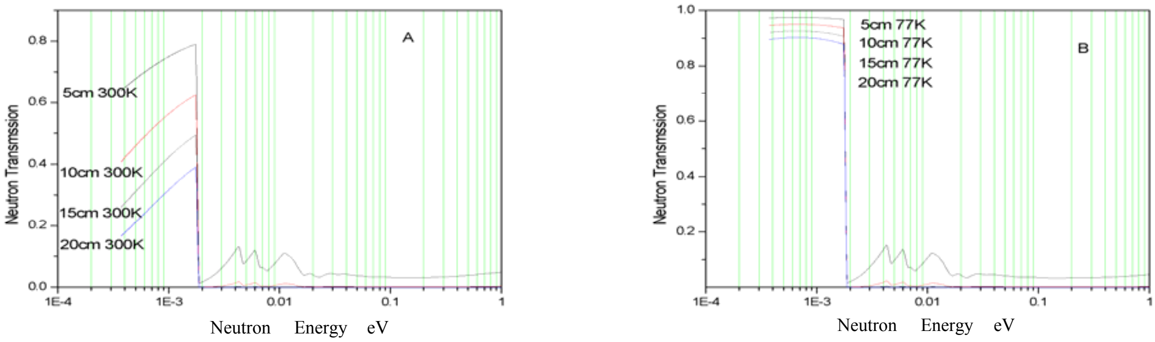

Fig. (6). Neutron transmission through polycrystalline graphite

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 Fig(7) before and after its transmission through the 10cm thick polycrystalline graphite cooled to 77K. It is observed that the 10cm graphite transmits about 90 % neutrons with wav … phite under these co … ons, while efficientl

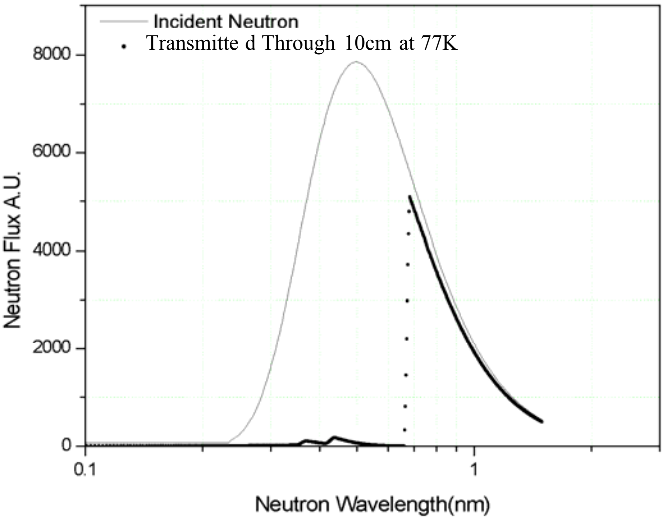

Fig. (7). Transmitted cold neutron flux through polycrystalline graphite

3.Polycrystalline iron

Using the COLDFILTER code, the total neutron cross-sections of Fe at 300 K were calculated for neutrons in the energy range from 1 meV up to 0.1 eV. The results of calculation for poly-crystalline iron in metal form with ρ = 7.8 gm/cc and in powdered one with ρ' = 5.4 gm/cc are displayed in Fig (8) as solid lines. For comparison, the experimental data for metallic iron reported by M. Adib [14] and those for powdered iron reported by Harvey [2] are also displayed in Fig (8).

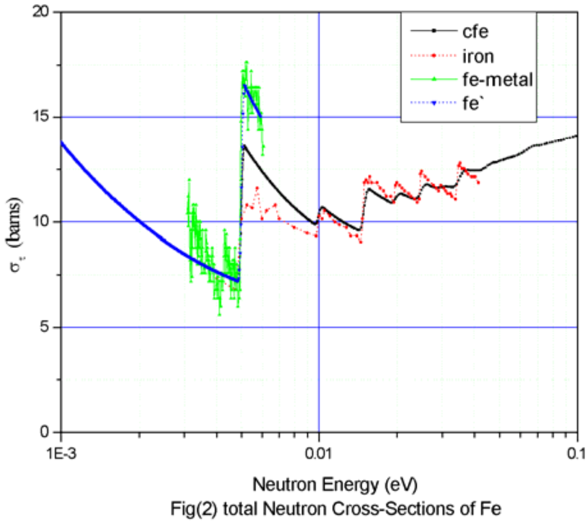

Fig. (8) Total neutron cross-section of Fe

The calculated results for both values of densities are in reasonable agreement with experimental ones, for the fitted parameters $C_2 = 0.4\ \text{nm}^{-2}.\ \text{eV}^{-1}$ and $\theta_D = 350$ K.

From Fig. (8), one can observe that Fe total cross-section beyond the cut-off wavelength $\lambda_c = 2d_{110} = 0.404$ nm (at E < 5.0 meV) reduced down to 7.0 barns from 12 barns at E > 1 eV. Thus it is worthwhile to carry out a feasibility study for the use of poly-crystalline iron as a cold neutron filter.

To show the effect of thickness of poly-crystalline iron on its filtering features, the calculation was performed at LN_2 (liquid nitrogen) temperature, for neutron wavelengths in the range from 0.01 nm up to 1.0 nm. The results of these calculations are displayed in Fig.(9). The indication is that 4.0 cm thick poly-crystalline iron cooled at LN_2 temperature transmits about 25% of incident neutrons with $\lambda > 0.4$ nm,

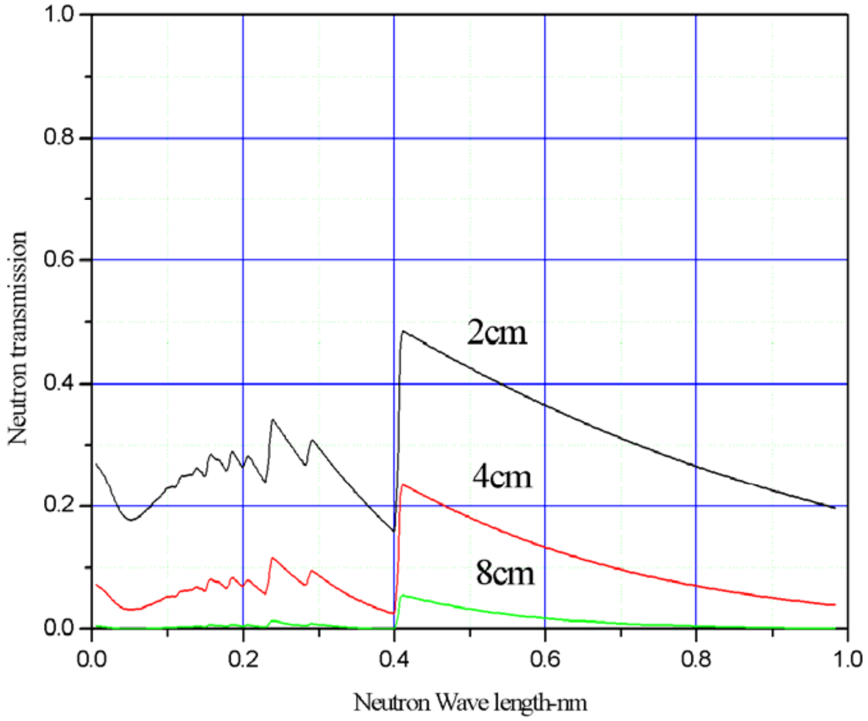

Fig. (9) Neutron transmission through different thickness of polycrystalline Fe

temperature transmits about 25% of incident neutrons with λ > 0.4 nm, transmission being 11% for neutrons close to 0.29 nm and 9% for λ close to 0.23 nm due to reflections from (200) and (211) planes respectively. The calculated cold neutron flux, for which there is a Maxwallian distribution, for a neutron gas temperature close to liquid hydrogen, is displayed in Fig.(10) before and after its transmission through a 4.0 cm thick of poly-crystalline iron cooled to 77 K. It is observed that the transmitted neutron intensity within the neutron wavelength band from 0.23 to 0.4 nm is less than one tenth of its value beyond the cut-off wavelength. Thus polycrystalline iron can be sufficiently used as a cold neutron filter rather than poly-crystalline Be [15], when the intensity of the γ-rays accompanying the neutron beam is relatively high.

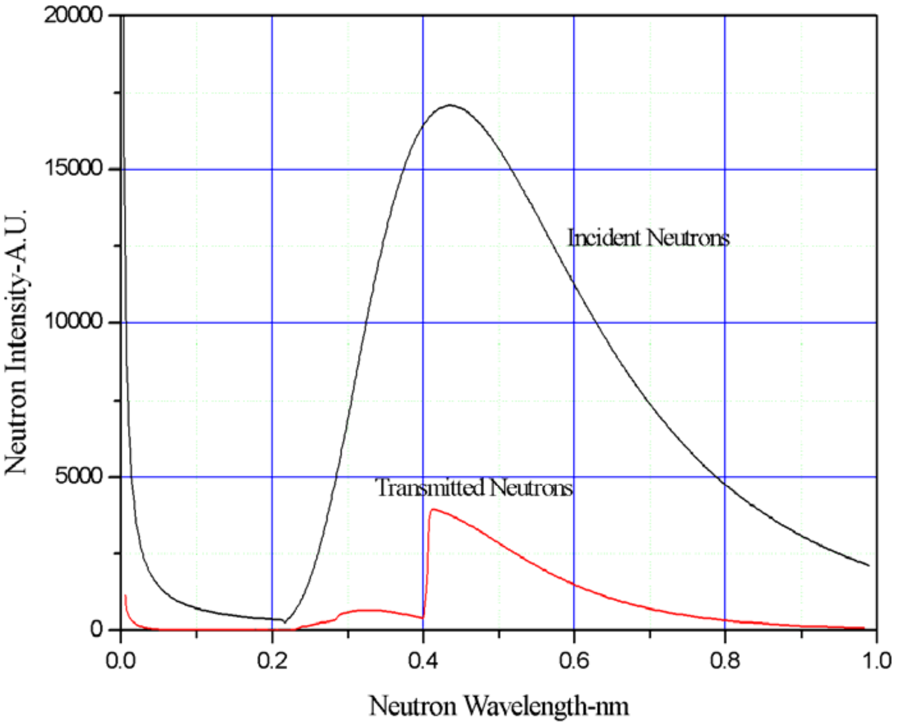

Fig. (10) Transmitted cold neutron flux through 4 cm Fe at LN_2

Conclusion

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

Calculations show that 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.

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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.

Moreover, polycrystalline iron can be sufficiently used as a cold neutron filter rather than poly-crystalline Be, when the intensity of the γ-rays accompanying the neutron beam is relatively high.

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