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Neutron Transmission Through Crystalline Fe

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Abstract: The neutron transmission through crystalline Fe has been calculated for neutron energies in the range $10^{-4} < E < 10$ eV using an additive formula. The formula permits calculation of the nuclear capture, thermal diffuse and Bragg scattering cross-section as a function of temperature and crystalline form. The obtained agreement between the calculated values and available experimental ones justifies the applicability of the used formula. A feasibility study on using poly-crystalline Fe as a cold neutron filter and a large Fe single crystal as a thermal one is given.

Key words: Thermal neutron filters, crystalline Fe

INTRODUCTION

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

Poly and mono-crystals now-a-days are commonly used as thermal neutron filter[1-4]. 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. Figure 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.

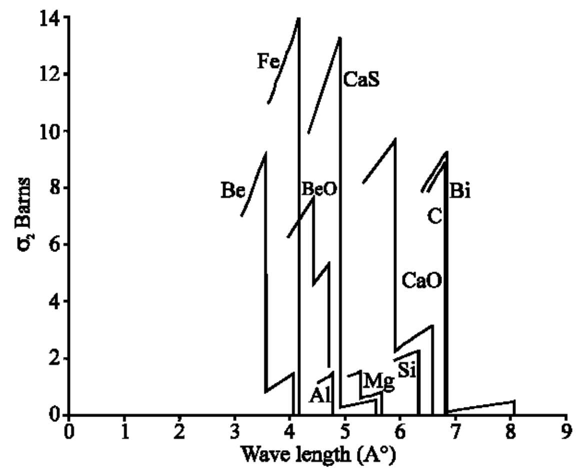

Fig. 1: The cross sections in the vicinity of the Bragg cot-off wavelengths for a nunber of poly-crystallin materials

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. Therefore, the present work deals also with the evaluation of using large Fe single crystal, as a thermal neutron filter since it has only two atoms per unit cell (body-centered cubic structure) with lattice constant a_o=0.286 nm consequently the positions of the reflected Bragg peaks are shifted toward short wavelengths and will not disturb the filtered thermal neutron beam of long wavelengths. Moreover Fe can be obtained as a large single crystal with small mosaic spread value.

Theoretical treatments: The total cross-section determining the attenuation of neutrons by crystalline iron can be given as:

$$\sigma = \sigma_{abs} + \sigma_{tds} + \sigma_{bragg} \quad (1)$$

where, the neutron capture cross-section σ_{abs} which obeys the $E^{-1/2}$ law can be written as $\sigma_{abs} = C_1 E^{-1/2}$ with E

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the neutron energy and C_1 is a constant which can be calculated from values provided by Sears[5]. The TDS cross-section σ_{tds} as a function of materials constants, temperature, total coherent scattering cross-section and neutron energy is given by Freund[6]. A constant C_2 which depend on atomic weight and the value of Debye temperature θ_D are suggested by Freund[6] as parameters, to fit the calculated cross-section to experimental ones.

The contribution of Bragg scattering σ_{Bragg} to the total cross-section takes into account the reflections from different (hkl) planes.

In case of poly-crystalline materials as shown by Bacon[7] σ_{Bragg} can be given as:

$$\sigma_{Bragg} = \frac{\lambda^2 N_c}{2} \rho'/\rho \sum_{d_{hkl}} M_{hkl} F_{hkl}^2 d_{hkl} e^{-2w} \tag{2}$$

where, N_c is the number of unit cell per cc , F_{hkl} is the structure amplitude factor per unit cell, θ_D the Debye Waller factor, M_{hkl} its multiplicity and ρ' and ρ are the densities of the powdered form used and its metallic one, respectively.

In case of single crystal materials, the Bragg scattering cross-section is given by Naguib and Adib[8] :

$$\sigma_{Bragg} = \frac{-1}{Nt_o} \ln \left[\prod_{hkl} (1 - P_{hkl}^{\theta}) \right] \tag{3}$$

where, N is the number of atoms cm^{-3} , t_o is the effective thickness of the crystal in cm. P^{θ}_{hkl} is the reflection power of the (hkl) plane inclined by an angle θ_{hkl} to the incident neutron beam direction.

As shown by Adib and Habib[9] the reflecting power $P^{\theta}_{hkl}$for an imperfect crystal depends upon both the direction cosine of the incident beam relative to the inward normal to the crystal surface γ_o , the direction cosine of the diffracted beam γ_{hkl} and the inclination of the (hkl) plane to the crystal surface α_{hkl}.

Iron crystallizes in a body-centered cubic (bcc) structure with lattice constant a_i=0.286 nm .There are two atoms per unit cell. These two atoms have the following coordinates (0,0,0,), and (1/2,1/2,1/2).Therefore, the Bragg reflections appear only for h+k+l=even.

Following Adib and Habib[9], let a large Fe single crystal cut along the plane with Miller indices ($h_c k_c l_c$) is fixed on a goniometer's table such that its surface is parallel to X-Y plane. let also, the angle between the neutron between beam direction and the direction [$h_c k_c l_c$] is Ψ, then

$$\gamma_o = \cos\Psi$$

And the direction cosine of the diffracted beam γ_{hkl} can be expressed as:

$$\gamma_{hkl} = \frac{(hh_c + kk_c + ll_c)\cos\Psi + l_c \left[\frac{hh_c + kk_c}{\sqrt{h_c^2 + k_c^2}} + \frac{l\sqrt{h_c^2 + k_c^2}}{l_c} \right] \sin\Psi}{\sqrt{h_c^2 + k_c^2 + l_c^2} \ x \ \sqrt{h^2 + k^2 + l^2}} \tag{4}$$

while the inclination angle α_{hkl} can be given by:

$$\cos\alpha_{hkl} = \frac{(hh_c + kk_c + ll_c)}{\sqrt{h_c^2 + k_c^2 + l_c^2} \ x \ \sqrt{h^2 + k^2 + l^2}} \tag{5}$$

If the cutting plane is (0 0 l_c), thus equation (4) becomes:

$$\gamma_{hkl} = \frac{l\cos\Psi + k\sin\Psi}{\sqrt{h^2 + k^2 + l^2}} \tag{6}$$

and equation (5) becomes:

$$\mathrm{Cos}\,\alpha_{hkl} = 1/\sqrt{h^2 + k^2 + l^2} \tag{7}$$

A computer code CFE (Crystalline Fe) has been developed in order to calculated the total cross-section and transmission of neutrons of energy range from 1 meV to 10 eV, incident on either poly-crystalline iron or large mosaic single crystal.

For comparison of the experimental neutron cross-section data with the calculated values, the program takes into consideration the effects of both neutron wavelength resolution and incident neutron beam direction of the experimental arrangement used. The resolution function was considered to have a Gaussian distribution where the FWHM of the wavelength spread $\Delta\lambda$ of the distribution was deduced from the conditions of the experimental arrangement.

Comparision with experiment: In order to check the applicability of the deduced formula and developed computer code CFE , the total cross-sections of crystalline Fe as a function of neutron energy, were the calculated and compared with the experimental ones. The main physical parameters required in these calculations are listed in Table 1.

Table 1: Physical parameters of iron

Atomic weight	55.85
Crystal structure	BCC
Lattice constant	a_o=0.286 nm
Metallic density	7.8 g cc^{-1}
Number of atoms per unit cell	2
Coherent scattering length b	9.45 fm
Absorption cross-section for thermal neutrons σ(E=0.025 eV)barn	2.56 barns
Total scattering cross-section	8.606 barns

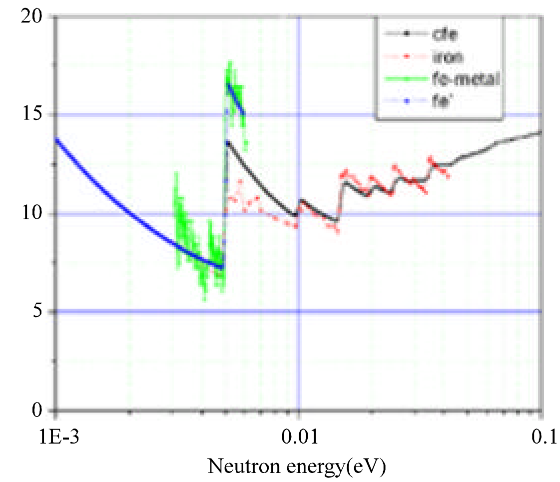

Fig. 2: Total neutron cross-sections of Fe

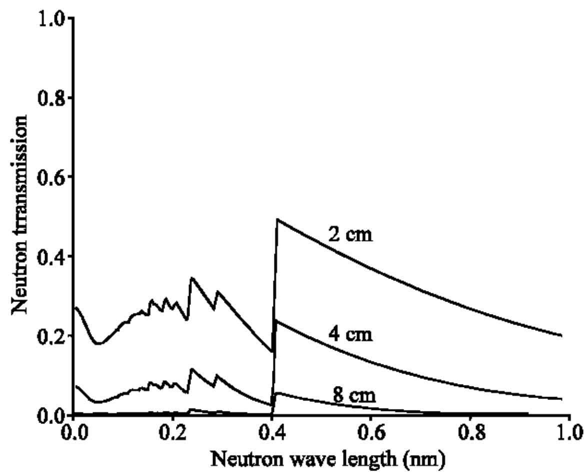

Fig. 3: Neutron transmission through different thickness of poly-crystalline Fe

Poly-crystalline iron: Using the CFE 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 g cc^{-1} and in powdered one with ρ'=5.4 g cc^{-1}are displayed in Fig. 2 as solid lines. For comparison, the experimental data for metallic iron reported by M. Adib[10] and those for powdered iron reported by Harvey[2] are also displayed in Fig. 2.

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

From Fig. 2, 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

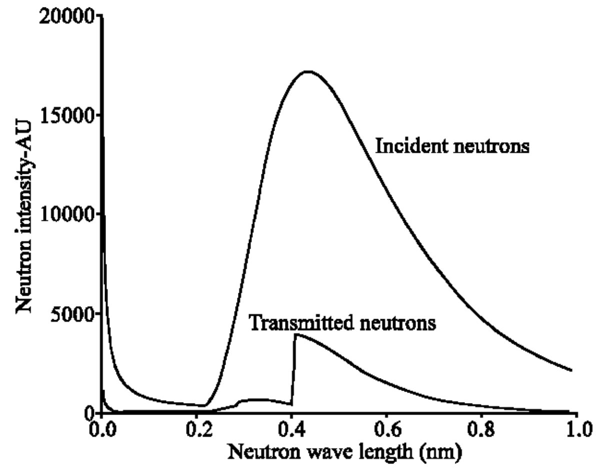

Fig. 4: Transmitted cold neutron flux through 4 cm Fe at LN_2

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. 3. The indication is that 4.0 cm thick poly-crystalline iron cooled at LN_2 temperature transmits about 25% of incident neutrons with λ>0.4 nm 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. 4 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[11], when the intensity of the γ-rays accompanying the neutron beam is relatively high.

Fe single crystal: In case of perfect single crystal the Bragg scattering term in Eq.(1) can be neglected. At neutron energies $\geq$1eV-binding effects of the atoms in solid can be neglected. Therefore, the total scattering is given by the free-atom cross-section and elastic scattering vanishes. As shown by Freund[6] with decreasing the neutron energy the multi-phonon scattering cross-section decreases while the single-phonon scattering and capture cross-section varies

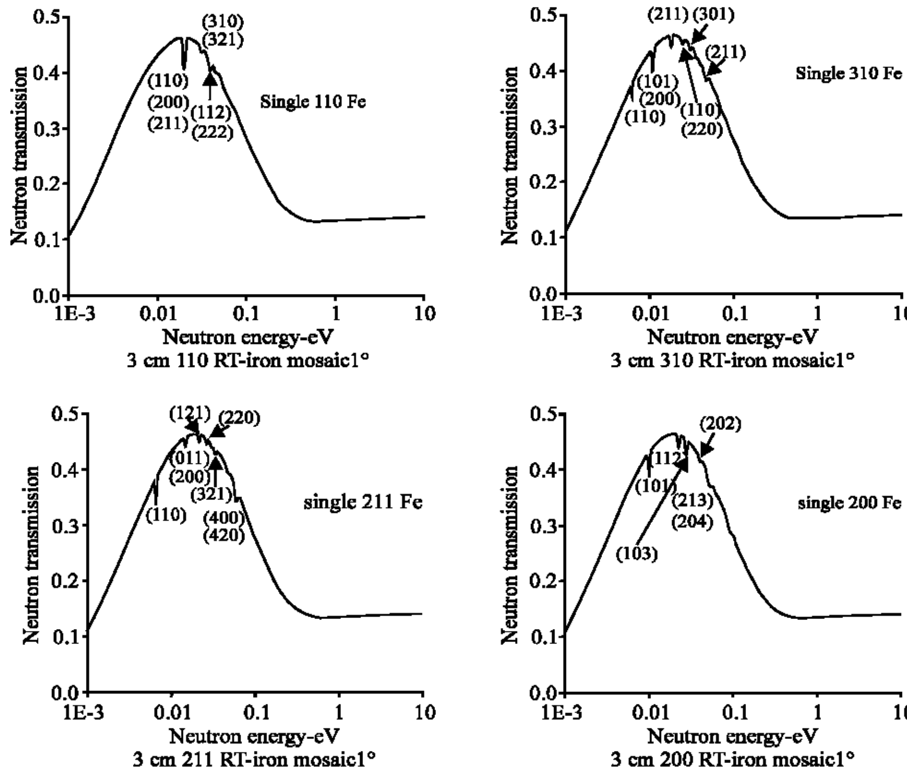

Fig. 5: Neutron transmission through Fe crystal cut along different planes

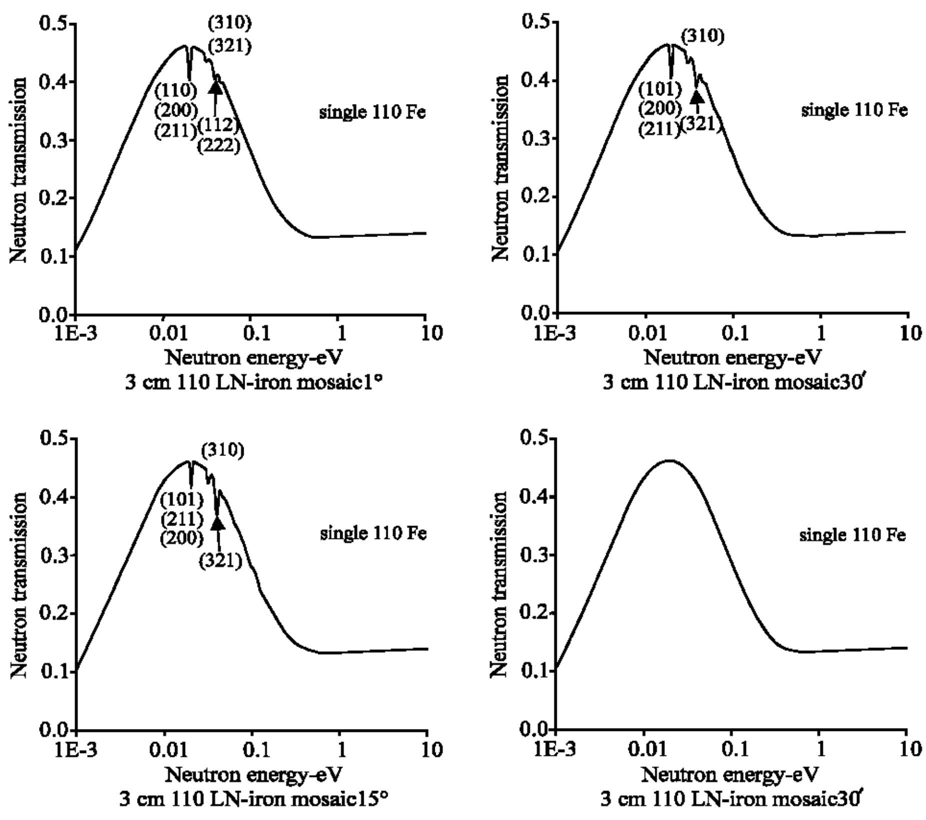

Fig. 6: Neutron transmission through 3 cm of Fe crystals for various mosaic models

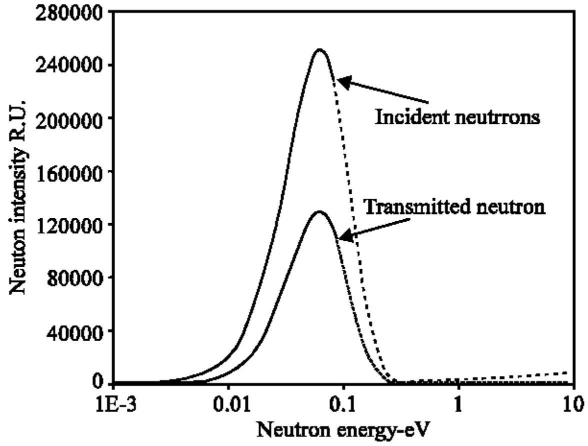

Fig. 7: Incident and transmitted thermal neutron flux through Fe single crystal

like $E^{-1/2}$. Therefore the total cross-section of Fe perfect single reaches a minimum cross-section value of 4.4 barn at E=0.02eV.This means that a 3 cm thick perfect iron single crystal attenuates neutron with energies>1 eV by a factor of 7.5 while the attenuation factor of neutrons around 0.02 eV is only 2.2. Such attenuation properties makes the use of perfect iron single crystal as a thermal neutron filter feasible. However the utilization of manufacturing a large perfect Fe single crystal is a very tedious and expensive job. Consequently, the contribution of the Bragg scattering to the total cross-section of imperfect Fe single crystal is not negligibly small. To show the contribution of the Bragg reflections on the transmitted through a 3 cm thick Fe single crystal, cutting along different (h_c k_c l_c) planes, calculations were performed using CFE code, assuming room temperature

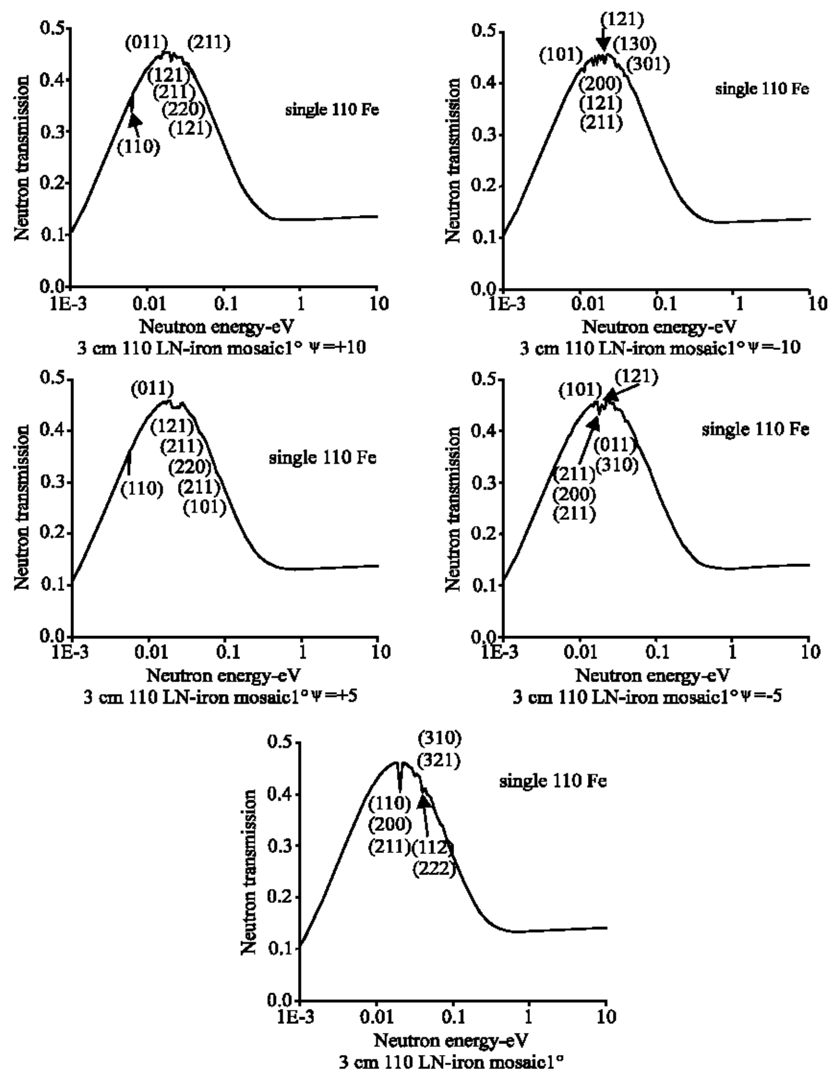

Fig. 8: Fine tunning of Fe single crystals cut along (110) plane

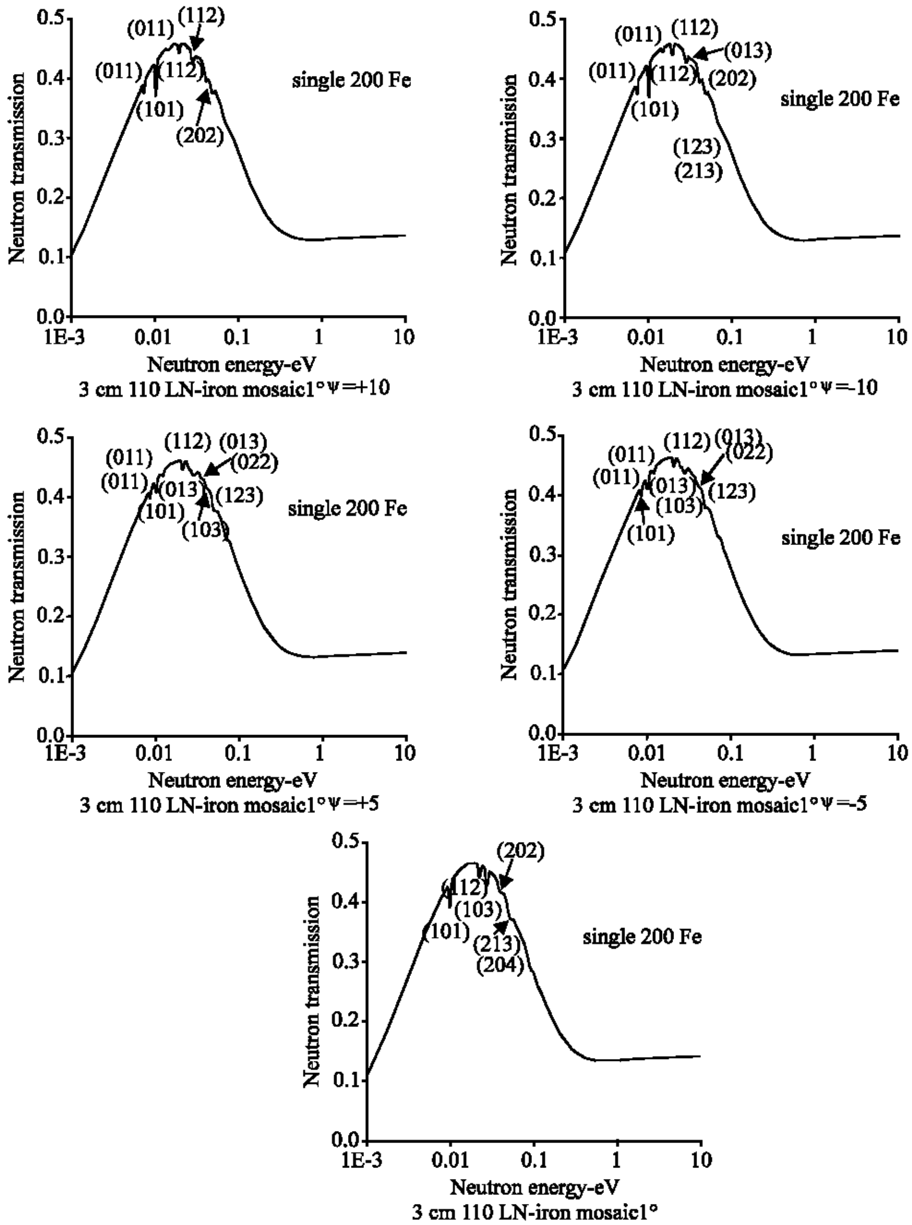

Fig. 9: Fine tunings of Fe single crystal cut along (200) plane

and crystals have the same FWHM of the mosaic spread of 1°.

Figure 5 displays the result of calculation for Fe crystals cut along (110), (200), (211) and (310) planes for neutrons incident perpendicular to the cutting plane i.e. at $\Psi=0$. It is apparent that, Fe crystal cut a long its (110) plane, when it used as a thermal filter, is preferable to other cuts, since no pronounced Bragg reflections occur for neutron energies <20 meV. To decrease Bragg reflections at neutron energies>20 meV, an optimum choice of the crystal mosaic speared is essential. Neutron transmission through a 3 cm thick Fe (110) crystal cooled to LN_2 temperature, for a different values of mosaic spread were calculated and displayed in Fig. 6. As may be observed for FWHM of mosaic spread>3 min of arc, parasitic Bragg reflections could limit the use of Fe as a thermal neutron filter. Figure 7 shows that a 3 cm thick Fe (110) crystal cooled to LN_2 temperature can be successfully used to transmits more than 50% of thermal neutron flux having a Maxwellian distribution with neutron gas temperature close to 300 K, while significant rejecting the a accompanying γ-rays and epithermal and fast neutron.

However, fine tuning of Fe crystal with mosaic spread>3′ (i.e., less expensive one) can reduce the effect of Bragg reflections. To show how to select the orientation, at each neutron energy, the neutron transmission through 3 cm Fe crystal (having mosaic spread of 1°) have been calculated as a function of neutron energy at different **Ψ** from -10° to 10°.The results of calculation are displayed in Fig. 8 and 9 for cutting plane (110) and (200), respectively. Such calculation shows that the tuning effect is asymmetric for (110) cutting plane, while it is symmetric for the (200) one. Therefore one may use such low quality Fe single crystals, as a sufficient thermal neutron filter. Moreover, it is obvious that tuning is sufficient within ±10° and the cutting along (200) plane is preferable that (110) since the tuning can be done regardless the direction of orientation.

CONCLUSION

Poly-crystalline 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.

The calculation shows that 3 cm thick iron single crystal cut a long its (110) plane, with a standard deviation on a mosaic spread of 3 min of arc, is a good thermal-neutron filter, with reasonable effect-to-noise ratio. While fine tuning of low quality iron single crystal cut a long its (200) plane can be used as a sufficient thermal neutron filter.

To improve the filtering characteristics of iron, one make use of iron oxides. Iron oxide is considered to be a better choice than iron, its Debye temperature and free atom scattering cross-section being higher than the later at the same value of their capture cross-section. The study of the filtering characteristics of Fe_2O_3 crystal is given elsewhere.

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