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Attenuation of Thermal Neutrons by Crystalline Silicon

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A simple formula is given which allows to calculate the contribution of the total neutron cross – section including the Bragg scattering from different (*hkl*) planes to the neutron transmission through a solid crystalline silicon. The formula takes into account the silicon form of poly or mono crystals and its parameters. A computer program DSIC was developed to provide the required calculations.

The calculated values of the total neutron cross-section of perfect silicon crystal at room and liquid nitrogen temperatures were compared with the experimental ones. The obtained agreement shows that the simple formula fits the experimental data with sufficient accuracy .A good agreement was also obtained between the calculated and measured values of polycrystalline silicon in the energy range from 5eV to 500μeV.

The feasibility study on using a poly-crystalline silicon as a cold neutron filter and mono-crystalline as a thermal neutron one is given. The optimum crystal thickness, mosaic spread, temperature and cutting plane for efficiently transmitting the thermal reactor neutrons, while rejecting both fast neutrons and gamma rays accompanying the thermal ones for the mono crystalline silicon are also given.

INTRODUCTION

A fission reactor is a prolific source of fast neutrons, thermal neutrons and gamma radiation . However , to improve the signal-to-background ratio for thermal neutron scattering experiments has required the development of thermal neutron filters .

For most media the reflective index for neutrons is less than 1.0. It follows that when a neutron beam strikes the boundary of a medium from out side (i.e. from vacuum) , one should observe an almost total internal reflection of neutrons from the surface at small enough glancing angles .As shown by several authors [1,5],that curved guide tubes transports neutrons by total internal reflection from a surface coating of ^{58}Ni mirror ,while reject both fast neutrons and gamma radiation. Therefore, such neutron guide tubes are now-a days used as thermal neutron filters.

Such thermal neutron filters are expensive to construct and the neutron scattering facility are usually installed far away from the reactor core .

However poly and momo-crystals have been recently used as thermal neutron filter[6,7].When evaluating crystal filters that pass thermal neutron and exclude both fast neutrons and γ-rays , the material used must be of small absorption cross-section and small diffuse scattering cross-section . Therefore the present work deals with the feasibility study on using a poly and mono-crystalline silicon as a thermal neutron filter.

A simple formula was introduced for calculating both the total thermal cross-section and Bragg scattering cross-section of a silicon in poly and mono crystalline form.

The computer program DSIC, a new version of computer code ISCANF- II was adapted to provide the required calculation.

THE THEORETICAL TREATMENT

1. Attenuation of thermal neutrons by a crystalline solid :

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

$$\sigma = \sigma_{abs} + \sigma_{tds} + \sigma_{Bragg} \tag{1}$$

The first contribution σ_{abs} for the most of the elements obeys the 1/v law where v is the neutron velocity and can be written as:

$$\sigma_{abs} = C_1 E^{-1/2} \tag{2}$$

where E is the energy of the incident neutron

Açcording to Freund [8] the second contribution σ_{tds} can be split into two parts, σ_{sph} and σ_{mph} depending on neutron energy. The single-phonon-scattering cross section σ_{sph} concerns the energy range $E \ll K_B \theta_D$, where K_B is Boltzmann' s constant and θ_D is the characteristic Debye temperature is given by the equation:

$$\sigma_{sph} = \frac{\sigma_{bat}}{36A}\left(\frac{\theta_D}{E}\right)^{1/2} \begin{cases} R & x \leq 6 \\ 3.3\,x^{-7/2} & x \geq 6 \end{cases} \qquad (3)$$

where $x = \theta_D/T$ (T is the temperature), $\sigma_{bat} = S + s$ the sum of coherent and incoherent scattering cross section of the bound atom, A is the atomic mass number and

$$R = \sum_{n=0}^{\infty} B_n\, x^{n-1} / [\, n\,!\, (n+5/2)]$$

where B_n are the Bernoulli numbers.

The second part, the multi-phonon scattering σ_{mph} of the σ_{tds} is predominant on the range $E \gg K_B\, \theta_D$ and is given by:

$$\sigma_{mph} = \sigma_{free}\ \{\, 1 - \exp[\, -(B_o + B_T)\, C_2\, E\,]\, \}$$

where C_2 is a constant independent of the scattering material,

$$B_o = 3\, h^2 / (2\, K_B\, \theta_D)$$

$$B_T = 4\, B_o\, \varphi(x)/x$$

in which h is plank's constant and

$$\varphi(x) = x^{-1} \int_0^x \zeta\ d\zeta / (e^{\zeta} - 1)$$

σ_{free} is the free atom cross section given by

$$\sigma_{free} = \sigma_{bat}\ [\ A/A+1]^2$$

2. Bragg Scattering :

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 $d_{hkl} \geq \lambda/2$, while in case of mono crystal, reflections are from the *(hkl)* planes satisfying the Bragg equation:

$$n\lambda = 2\, d_{hkl} \sin \theta_{hkl}$$

where n is the order of reflection, θ_{hkl} is the glancing angle to the *(hkl)* plane.

2. 1. Bragg Scattering by a Polycrystalline Material:

It was shown by Bacon [9] that for a Polycrystalline material with grain size less than 10^{-4} mm, the total coherent Bragg scattering cross-section can be given as:

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

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.

2. 2. Bragg Scattering by Single Crystal:

Following Naguib K. and Adib M., [10], the Bragg scattering cross-section by a single crystal is given by:

$$\sigma_{\text{Bragg}} = \frac{1}{N t_o} \ln\left(\frac{1}{T_{Bragg}}\right) \tag{5}$$

where N is the number of atoms per cubic centimeter and t_o is the effective thickness of the crystal in cm. T_{Bragg} is the resulting neutron transmission from different (*hkl*) planes given by:

$$T_{\text{Bragg}} = \prod_{hkl} \left(1 - P_{hkl}^{\theta}\right)$$

where P_{hkl}^{θ} is the reflecting power of the (*hkl*) plane inclined by an angle θ_{hkl} to the incident beam direction.

As shown by Naguib K. and Adib M., [10] the reflecting power P_{hkl}^{θ} for an ideally imperfect crystal depends upon the direction cosine of the incident beam γ_o relative to the inward normal to the crystal surface cutting along the plane $(h_c k_c l_c)$, the direction cosine of the diffracted beam γ_{hkl} and the inclination of (*hkl*) plane to the crystal surface α_{hkl}.

For the diamond cubic structure, the equation describing the cutting plane $(h_c k_c l_c)$ which is parallel to the crystal surface can be given as:

$$\sqrt{h_c^2+k_c^2+l_c^2}\ \ Z = a_o$$

while any of the *(hkl)* planes can be given as:

$$\frac{1}{\sqrt{h_c^2+k_c^2}}\left(hk_c-kh_c\right)\ X + \left[\frac{l_c}{\sqrt{h_c^2+k_c^2+l_c^2}}\left(\frac{hh_c+kk_c}{\sqrt{h_c^2+k_c^2}}-\frac{l\sqrt{h_c^2+k_c^2}}{l_c}\right)\right] Y +$$

$$+\ \frac{hh_c+kk_c+ll_c}{\sqrt{h_c^2+k_c^2+l_c^2}}\ Z = a_o \qquad (6)$$

where a_o is a lattice constant.

Let the angle between the neutron beam direction and the direction $[h_ck_cl_c]$ is ψ, then the direction cosine of the diffracted beam γ_{hkl} can be expressed as:

$$\gamma_{hkl} = \frac{\left(hh_c+kk_c+ll_c\right)\cos\psi + l_c\left(\frac{hh_c+kk_c}{\sqrt{h_c^2+k_c^2}}-\frac{l\sqrt{h_c^2+k_c^2}}{l_c}\right)\sin\psi}{\sqrt{h_c^2+k_c^2+l_c^2}\ .\sqrt{h^2+k^2+l^2}} \qquad (7)$$

while the inclination angle α_{hkl} of any plane *(hkl)* to the cutting plane $(h_ck_cl_c)$ can be given as:

$$\cos\alpha_{hkl} = \frac{\left(hh_c+kk_c+ll_c\right)}{\sqrt{h_c^2+k_c^2+l_c^2}\ .\sqrt{h^2+k^2+l^2}} \qquad (8)$$

If the cutting plane is $(00l_c)$ equations (7) will be:

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

Description of DSIC Code

DSIC code is an adapted version of ISCANF-I and ISCANF-II codes developed to calculate the total neutron cross-section and transmission through crystalline material for neutron energies below 10 eV [11]. The contribution of σ_{abs}, and σ_{tds} are calculated in similar way as given in ISCANF-I and ISCANF-II programs. The adapted version DSIC can provide additionally the following calculations:

1-The nuclear unit-cell structure factor and the reflecting power P_{hkl}^{θ} of a diamond structure with 8 atoms per unit cell.

2-The energy and wavelength distribution of incident reactor neutron flux before and after its transmission through the crystalline filter, where the reactor neutron flux distribution was assumed to have 1/E for neutron energies E more than epithermal ones and Maxwellian with neutron gas temperature 300K or 77K for thermal or cold neutrons respectively .

Comparison with Experiment

In order to check the applicability of the deduced formula, the calculations were carried out for poly and mono crystalline silicon crystals and compared with the experimental ones. The main silicon physical parameters used for calculations are listed in Table 1

Table .1 The physical properties of Silicon

Atomic Weight	28.08
Crystal Structure	Diamond Structure
Lattice Constant	a_o = 054307 nm
Atomic Positions	0 0 0, ½ ½ 0, ½ 0 ½ , 0 ½ ½ , ¼ ¼ ¼, ¾ ¾ ¼ , ¾ ¼ ¾ , ¼ ¾ ¾
Number of Unit Cells/m3	0.6243E+28
Debye Temperature	420K
Neutron capture cross-section at 0.025 eV	0.161 barns
σ_{bat}	2.180 barns
Coherent Scattering	4.2 fm

1. Polycrystalline Silicon

The total neutron cross-section of silicon was calculated in the energy range from 0.1 meV up to 10 eV using DSIC. The result of calculation was displayed in Fig. 1 as solid line. For comparison the available experimental values measured for polycrystalline silicon in powder form and reported in Refs 6&12 were also displayed in Fig. 1 . The calculated values are in reasonable agreement with the experimental ones at the fitted parameter C_2=6.4 . This value is close to that value 6.36 deduced from the semi empirical formula reported by Freund [8] .

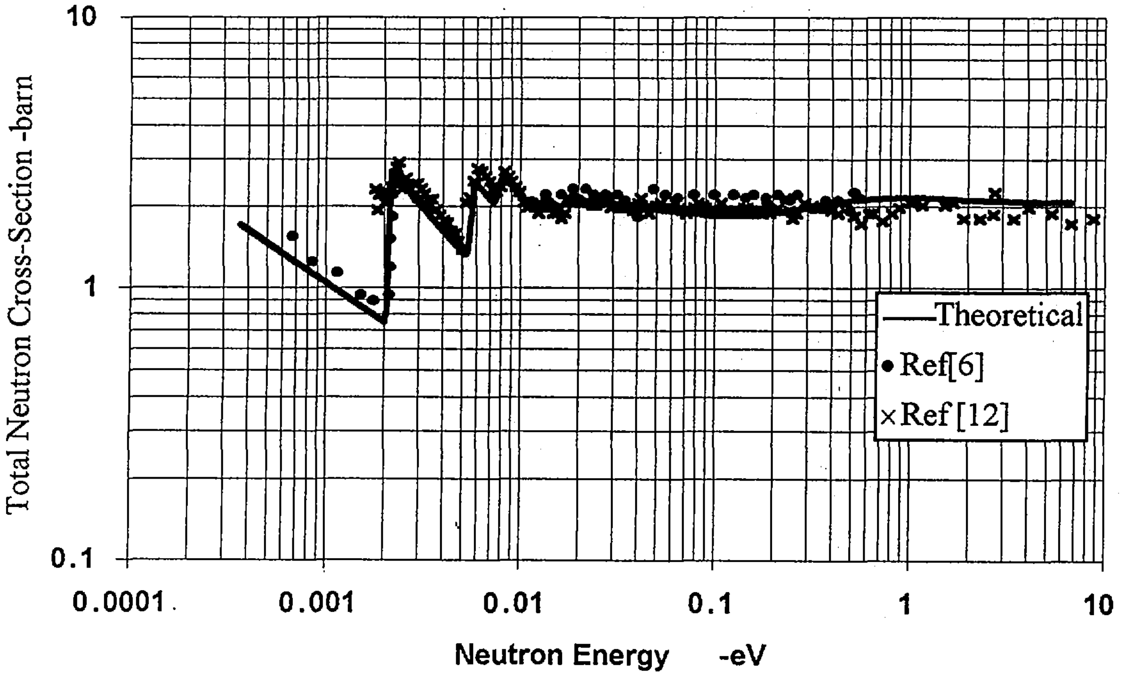

Fig .1 The Total Neutron Cross-Section For Polycrystalline Silicon .

To show the effect of both thickness and temperature of the polycrystalline silicon on its filtering characteristics, the calculations were performed at room and liquid nitrogen temperatures in the energy range from 1 meV up to 10 eV. The result of calculation is displayed in Fig. 2. It seems that 40 cm thick polycrystalline Si cooled at liquid nitrogen temperature has a better signal to background ratio for neutrons with wavelengths longer than the cut off wavelength at 0.628nm .

The calculated cold neutron flux having Maxwellian distribution with neutron gas temperature close to liquid Hydrogen (~ 20° K) incident on a 40 cm thick polycrystalline silicon cooled at liquid nitrogen before and after its transmission is displayed in Fig.3 .

Fig. 3 shows that 40cm of silicon transmits about 31% of the incident neutrons with wavelengths longer than 0.628nm. However it transmits about 9% for neutrons with wavelengths close to 0.38 nm,due to the reflection from (202) plane. Its seems that 40cm thick polycrystalline silicon cooled at liquid nitrogen is sufficient of almost removing epithermal neutrons and transmits less than 1% of fast ones with energies more than 1 MeV and less than 5% of γ-rays with energy $E\gamma = 2$ MeV, while,providing reasonable intensity of thermal neutrons (31%). Such transmission behavior limits the application of polycrystalline silicon when it used as a cold neutron filter.

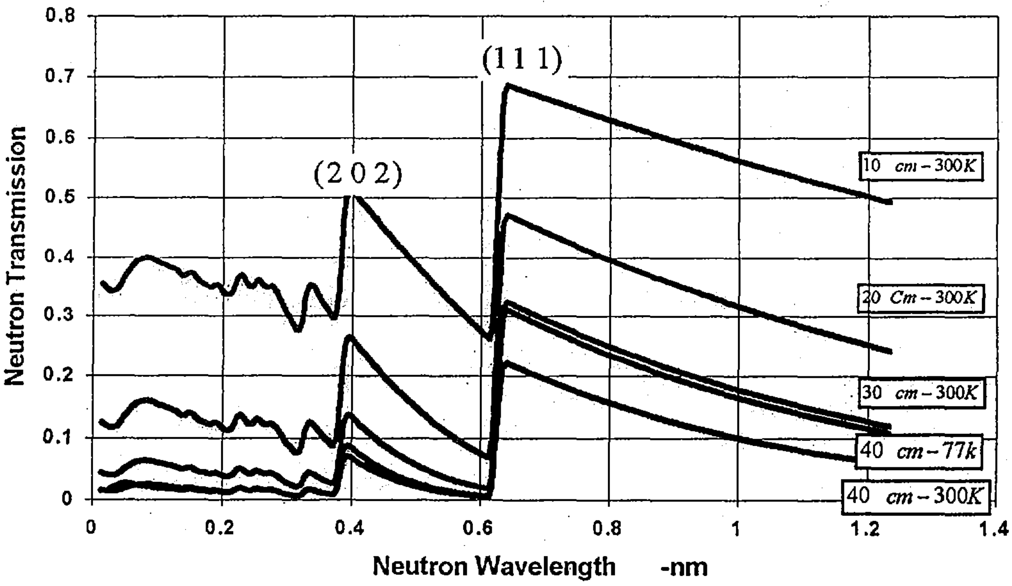

Fig.2 Neutron Transmission through different thickness Polycrystalline Silicon .

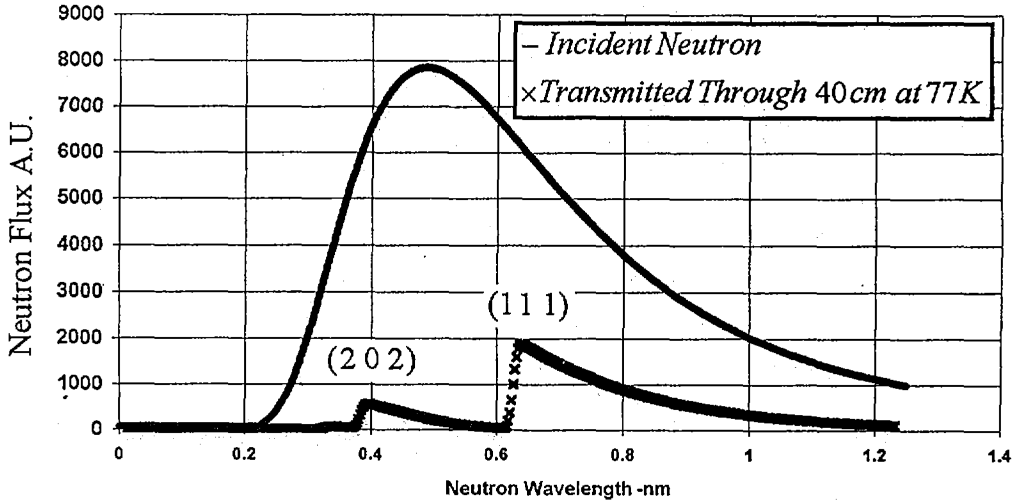

Fig.3 Transmitted Cold Neutron Flux through Polycrystalline Silicon .

Silicon Single Crystal :

The total neutron cross-section data carried out by Brugger[6] at both room and liquid nitrogen temperatures are displayed as dots in Fig.4a & b respectively . The calculated values using DSIC are also displayed in Fig.4 as solid lines assuming that Si single crystal is perfect and the neutron incident perpendicular to the (111) plane .

One can notice that the calculated values are in good agreement with the experimental ones. However as reported by Brugger[6]the neutron Bragg reflections from the crystal were smoothed by slightly titling crystal around zero inclination angle during the measurements.

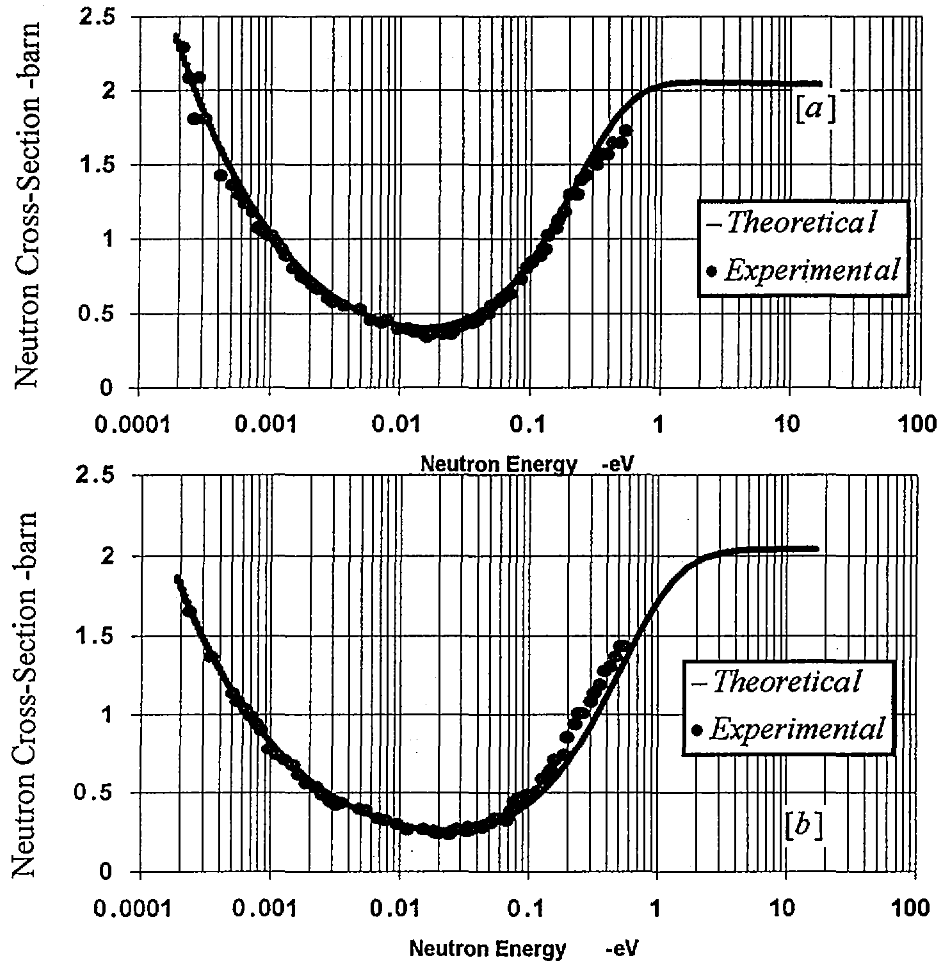

Fig .4 Neutron Cross-Section of a Perfect Si Single Crystal .

In order the check the effect of crystal mosaic spread on the neutron attenuation, the calculations were carried out assuming that 30cm Si single crystal is cut along (111) plane and cooled at liquid nitrogen temperature at different mosaic spreads. Fig.5 displays the result of calculation .From the figure one can notice that the Bragg reflections can not be neglected at mosaic spread values higher than 0.5mRad .

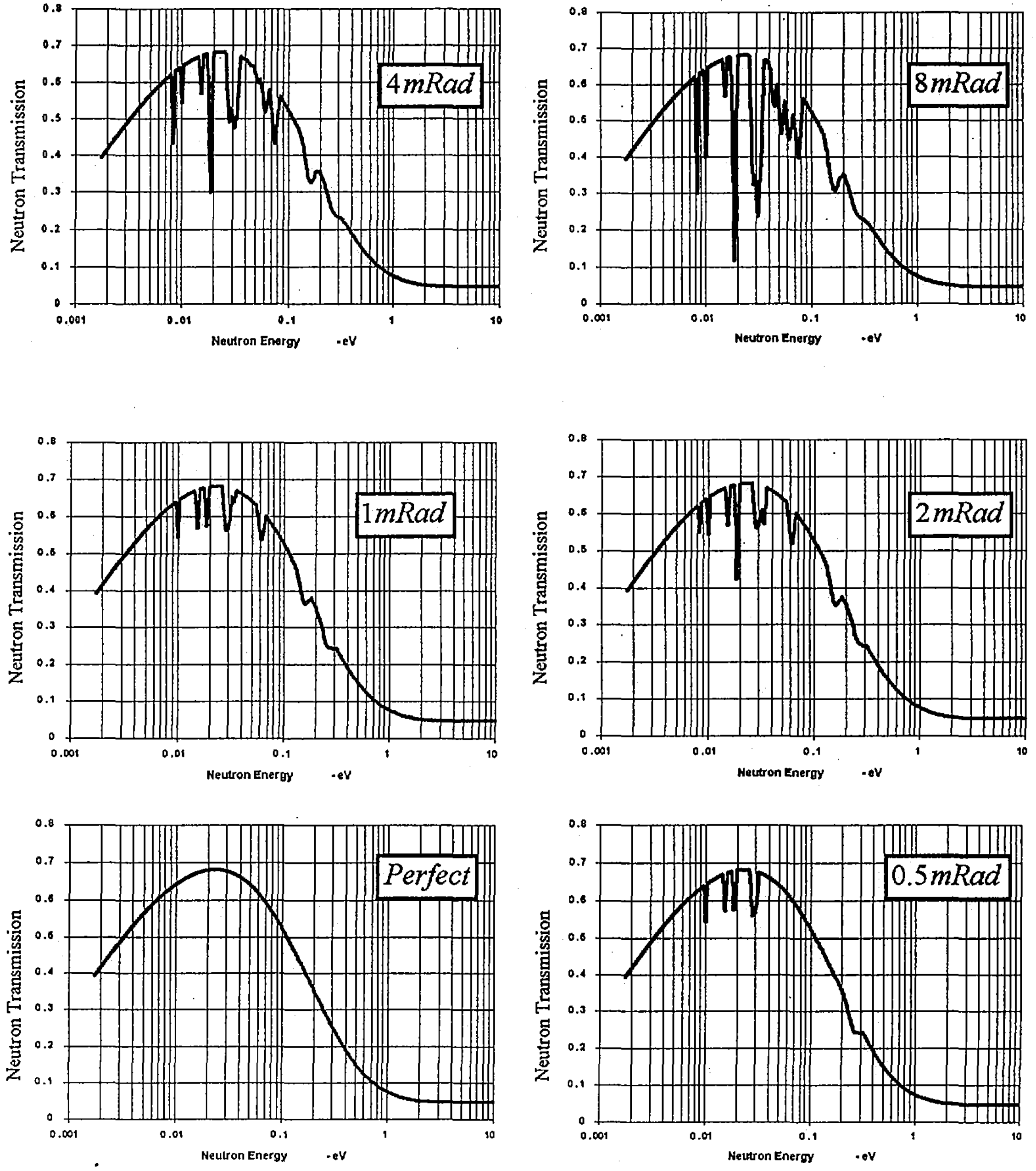

Fig.5. The Neutron transmission through 30cm of Si crystal for various mosaic spreads

To show the contributions of the Bragg reflections on the transmitted neutron spectra through also 30cm silicon single crystals cutting along different ($h_c k_c l_c$) planes and at room temperature, the calculations were performed in the whole energy range from 1 meV to 10 eV and assuming that their mosaic spread are the same and have the value of 4mRad. Fig. 6 displays the results of calculation for neutron transmission through silicon crystals cut along, (331), (311), (202), (002) and (111)planes at $\psi = 0°$. From the curves one can notice that the silicon crystal cut along (111) plane is preferable than others when it is used as a thermal neutron filter, since there is no disturbing Bragg reflections at neutron energies less than 0.01 eV

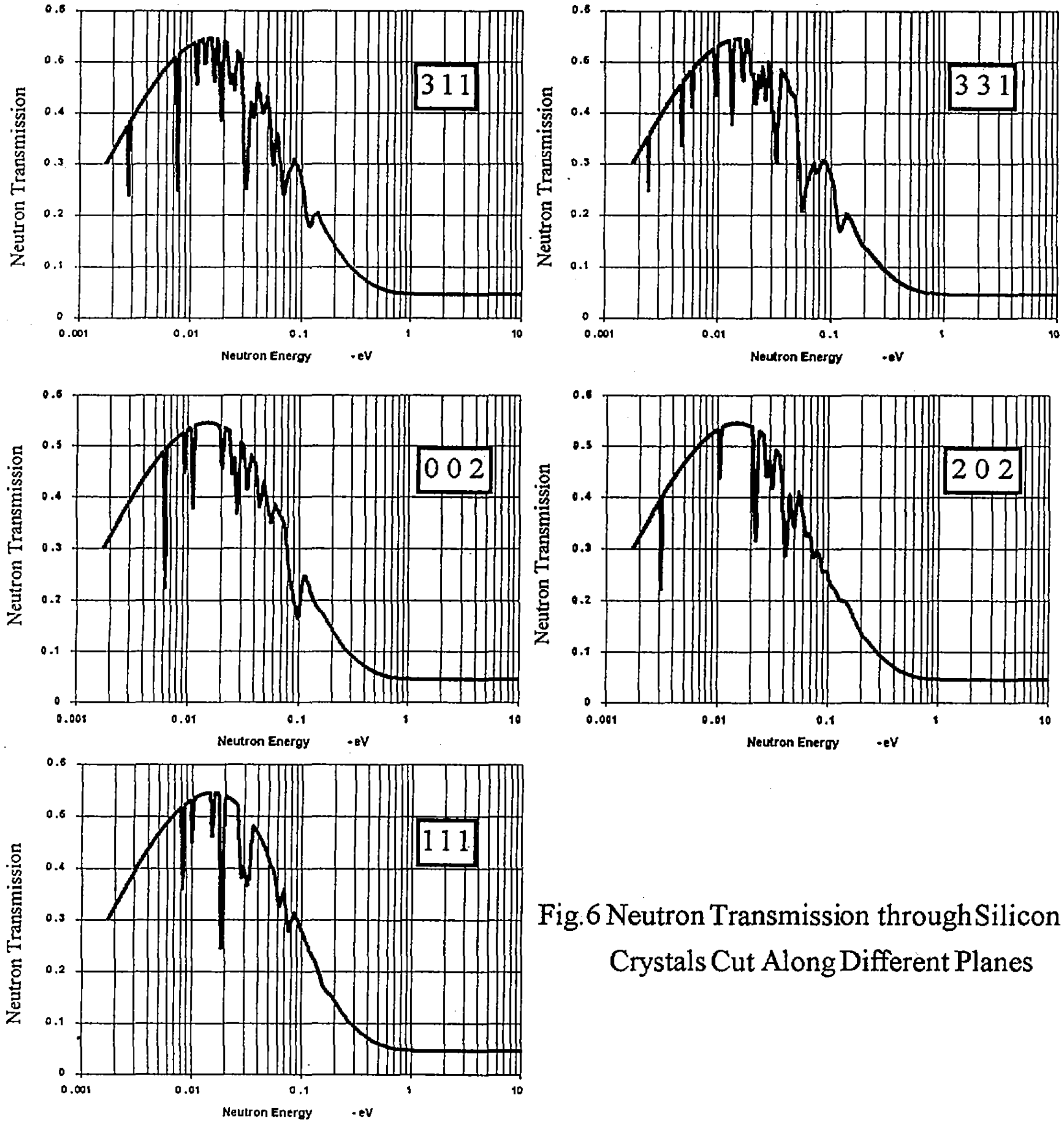

Fig.6 Neutron Transmission through Silicon Crystals Cut Along Different Planes

To find the optimum thickness of silicon (111) crystal, the neutron transmission~~s~~ ~~were~~ was calculated assuming that the mosaic spread has the value of 0.5mRad and 1mRad where the crystal was cooled at liquid nitrogen temperature. Fig.7a & b display the results of calculation for silicon single having mosaic 0.5mRad and 1mRad respectively . It seems that a 30 cm thick crystal with mosaic spread of 0.5mRad and cooled at liquid nitrogen temperature is free from parasitic Bragg reflection

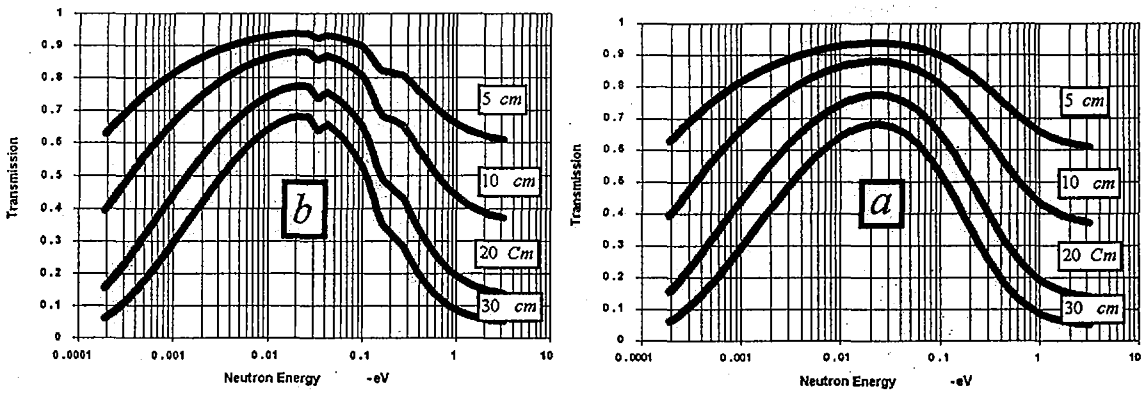

Fig.7 Neutron Transmission through silicon Crystals Cut along (111) Plane for Different Crystal Thickness

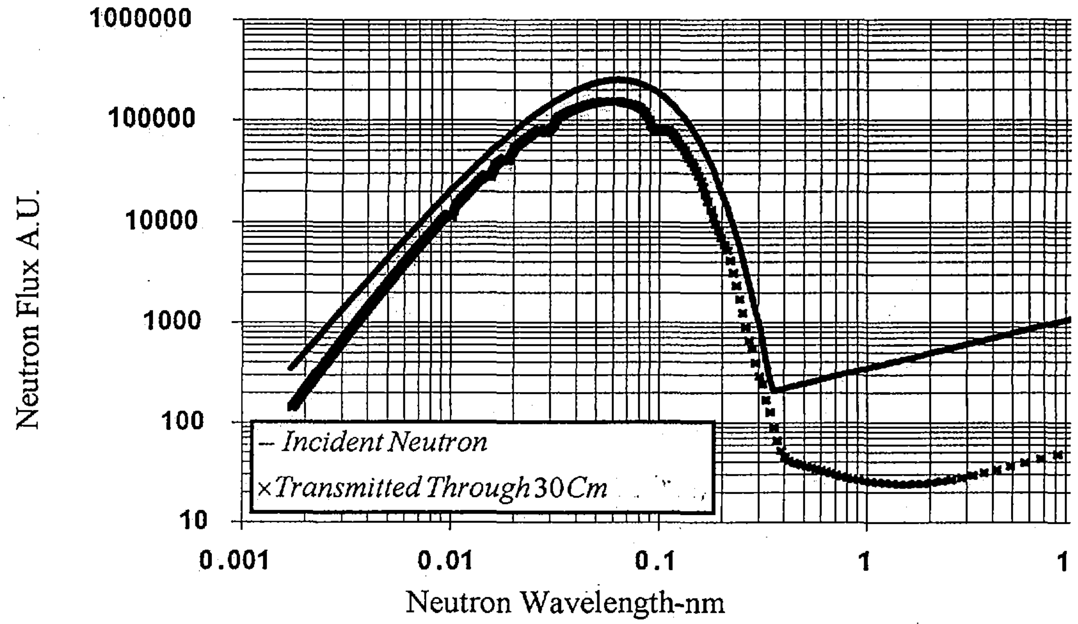

Fig.8 Transmitted Thermal Neutron Flux through Single Silicon Crystal cut along (111) Plane.

To show that such silicon crystal can be successfully used as thermal neutron filter the calculation of the transmitted thermal neutron flux through 30 cm silicon was carried out . The result of calculation is displayed in Fig.9 Where the thermal neutron flux was assumed to have a Maxwellian distribution with neutron gas temperature close to 300 K ,while the fast neutron one to have dE/E, where E is the neutron energy .

Its seems that 30 cm thick single crystal cooled at liquid nitrogen it sufficient of almost removing epithermal neutron and transmits less than 1% of fast ones with energies ~1 Mev and less than 5% of γ-rays with average energy Eγ =2 Mev while, providing reasonable intensity of thermal neutrons .

Such silicon single crystals now a days are commonly used to reduce the background of the high resolution powder diffractometers at both high flux reactors[4] and SINQ[5] .

CONCLUSION

The simple formula presented in this paper permits the calculation of the total cross-section of poly- and mono Si crystals with diamond structure to be deduced within an accuracy which is sufficient for determining the validity of such a crystal when it used as a thermal neutron filter. Calculations showed that polycrystalline silicon could be used as cold neutron filter while single crystal as a good thermal one at low γ-ray and fast neutron background .

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