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ABSTRACT

Using the IEA crystal spectrometer, the total neutron cross section of a Germanium single crystal was measured, for neutron energies between 1.0 to 0.01 eV, with the incident beam reaching the (111) planes perpendicularly.

The energy behavior of the Ge(111) effective absorption coefficient has been obtained through a comparison between calculated curves of total cross section and the experimental results. The value $\Theta = 370°K$ for the Ge Debye temperature was chosen among the several existing values for Ge.

I - INTRODUCTION

The calculation of the reflectivity of a crystal set of planes (hkl) requires the knowledge of the crystal effective absorption coefficient(1). If a narrow beam of monochromatic radiation passes through a thickness t of the crystal, the emergent intensity I is related to the incident intensity I_o by

$$I = I_o \, e^{-\mu t} \qquad (1)$$

Assuming that the crystal is oriented to avoid a Bragg reflexion of the monochromating planes, μ represents the effective absorption coefficient.

When a set (khl) of planes of the crystal is being used as monochromator, Bragg reflexions are produced by elastic coherent scattering; the effective absorption coefficient should include all interactions, other than Bragg scattering, that would take the neutron out of the incident or diffracted beam(2). Hence,

μ is the total macroscopic cross section of the single crystal, but with no consideration about the elastic coherent scattering of the monochromating planes (hkl).

The total macroscopic cross section Σ_T is composed of the absorption term Σ_a and the scattering term Σ_s.

$$\Sigma_T = \Sigma_a + \Sigma_s \qquad (2)$$

The Σ_a term is equal to $N\sigma_a$, where N is the number of atoms per cm^3 of the crystal, and σ_a is the capture microscopic cross section with an energy dependence proportional to $E^{-1/2}$.

All types of scattering are included in the Σ_s term as follows:

$\sum_{el}^{coh}$ - elastic coherent

$\sum_{inel}^{coh}$ - inelastic coherent

$\sum_{el}^{inco}$ - elastic incoherent

$\sum_{inel}^{inco}$ - inelastic incoherent

So eq.(2) may be rewritten as

$$\sum_T = N\sigma_a + \sum_{el}^{coh} + \sum_{inel}^{coh} + \sum_{el}^{inco} + \sum_{inel}^{inco} \qquad (3)$$

In a polycrystalline specimen, no elastic coherent scattering is possible at wavelength longer than twice the largest lattice spacing. However, since all crystalline orientations are possible, neutrons having wavelengths shorter than this cutoff wavelength will eventually satisfy the Bragg condition and elastic coherent scattering will occur[2].

For a single crystal, however, all crystalline orientations are not possible, and the Σ_{el}^{coh} contributions to the total cross section of the crystal occurs only at some determined energies. These contributions, which appear in form of peaks in the curve of Σ_T, are provided by Bragg reflexions of some determined crystalline planes. Except for these peaks, the energy dependence of the curve that represents Σ_T is described by the resulting curve obtained from the composition of the other types of cross sections.

The Σ_{el}^{coh} contribution form these crystalline planes will not be considered, since the present work main interest is to estimate the parameters involved in the calculations of the partial cross sections, which vary continuously with the neutron energy.

By an analysis of the remaining terms of eq. (3), one can affirm that, although both Σ_{el}^{inco} and Σ_{inel}^{inco} are strongly energy dependent, their sum is relatively constant[3], and over the energy range of thermal neutrons a reasonable approximation is[4,5]

$$\Sigma_{total}^{inco} = N\sigma_i = \Sigma_{el}^{inco} + \Sigma_{inel}^{inco} \qquad (4)$$

where σ_i is the incoherent microscopic scattering cross section of a single nucleus.

The inelastic coherent cross section Σ_{inel}^{coh} can be calculated using the Placzek "incoherent approximation"[6,7], which has been shown to be in agreement with experimental results in the energy range 0.001 to 1.0 ev[4], provided that the Debye temperature is properly chosen[5]. In this approximation the energy dependence is similar for the inelastic coherent and the inelastic incoherent cross sections, and σ_i is substituted by σ_c in the calculation of Σ_{inel}^{coh} : σ_c being the nuclear coherent microscopic scattering cross section.

$$\Sigma_{inel}^{coh} = (\frac{\sigma_c}{\sigma_i}) \Sigma_{inel}^{inco} \qquad (5)$$

Eq. (5) can be written in the form:

$$\Sigma_{inel}^{coh} = \frac{\sigma_c}{\sigma_i} (\Sigma_{total}^{inco} - \Sigma_{el}^{inco}) \qquad (6)$$

Using eq.(4) and the expression for Σ_{el}^{inco} that was used in several works[4,5,8], one can write

$$\Sigma_{inel}^{coh} = N\sigma_c \left[1-(1-e^{-\tau})/\tau \right] \qquad (7)$$

with $\sigma_c = 4\pi b^2$, where b is the nuclear scattering amplitude.

The function τ is given by

$$\tau = (\frac{24\ E\ m'}{k\ \Theta\ m}) \left[\frac{1}{4} + (\frac{T}{\Theta})^2 \ .\ \Lambda\ (\frac{\Theta}{T}) \right]. \qquad (8)$$

In eq.(8), E is the neutron energy, m' is the mass of the neutron, k is Boltzmann's constant, Θ is the Debye temperature of the crystal, m is the mass of the crystal atom, $\Lambda\ (\frac{\Theta}{T})$ is the Debye function and is expressed by

$$\Lambda\ (Z) = \int_0^Z \frac{x}{e^x-1} dx, \qquad (9)$$

T being the absolute temperature of the crystal.

Based on eq.(3), the effective absorption coefficient can be identified with the total macroscopic cross section Σ_T, as long as are neglected the peaks that arise from the elastic coherent scattering[2]. Eq.(3) can be rewritten in the following way:

$$\mu = N\sigma_T = N \left[\sigma_a + \sigma_i + \sigma_c \left[1- (1-e^{-\tau})/\tau \right] \right] \qquad (10)$$

With the aim of obtaining the energy behavior of μ, in a case of Bragg reflexions from a set of (111) planes of a Ge neu tron crystal monochromator, the total microscopic cross section, σ_T, of this crystal was measured.

II - EXPERIMENTAL RESULTS

The Instituto de Energia Atômica swimming pool research reactor operated at 2 Mw was the source of neutrons for this work. The transmission through the Ge crystalline sample was measured using the IEA crystal spectrometer[9,10].

The Ge crystalline sample was grown by the Semi-Elements Incorporated of Saxouburg, Pennsylvania, and has a disc shape with diameter 7,62 cm and thickness 1,51 cm. The crystal is oriented with the (111) planes parallel to the faces, and when the crystal is used as a monochromator the Bragg reflexions occur in the face.

However, in the present case, this crystal was used as a sample and the measurements were made with the incident neutron beam reaching the crystal perpendicularly to the face: this crystal position avoids the Bragg reflexions of the (111) planes and allows only the observation of the other interactions.

Figure 1 shows the experimental points of the total cross section, σ_T, of the crystal *versus* neutron energy: the small peaks in some determined energies are contributions of the $\sum_{el}^{coh}$ from crys talline planes other than (111).

The σ_T curve, calculated by eq.(10), must be confronted with the experimental points under the peaks, since in this equation the elastic coherent scattering was not considered.

In the Ge case, there are several measured values for the Debye temperature[11]. Therefore, the total microscopic cross sections were calculated with the following values of θ: 290°K, 354°K, 370°K and 390°K: the σ_T resulting curves are shown in figu

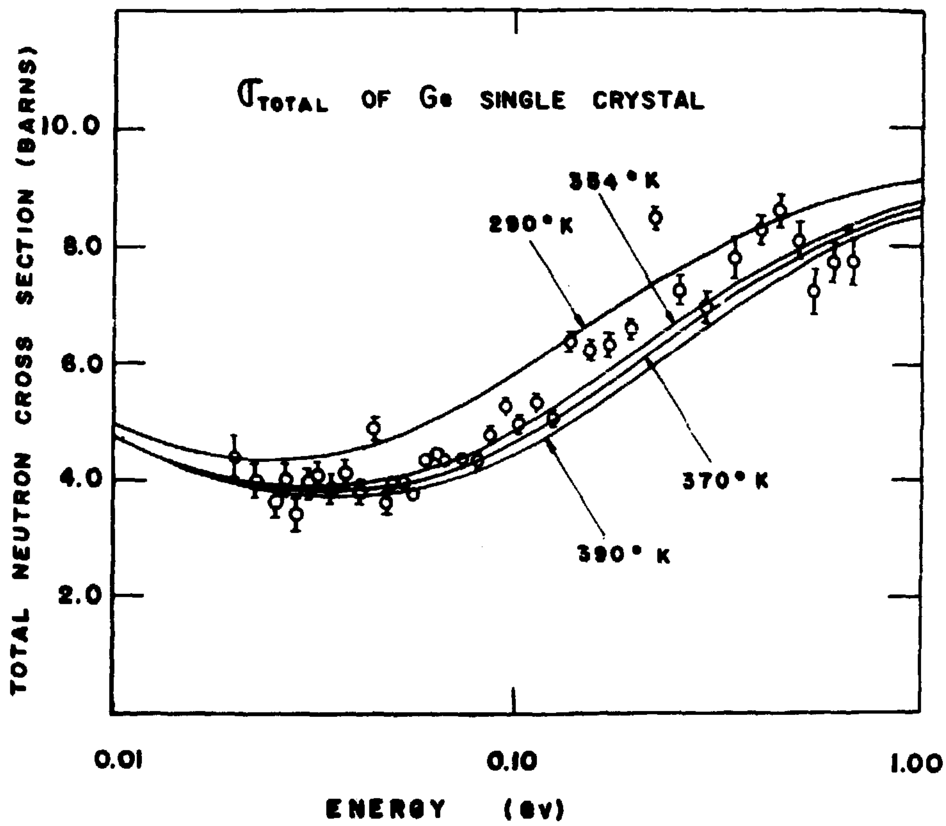

FIGURE 1 — Total neutron cross section of a Germanium single crystal. In the transmission measurements the incident beam was perpendicular to the (111) planes.

re 1. The comparison between the experimental points of the peak's base and the calculated curves, indicates that $\Theta = 370^{o}K$ is the suitable Debye temperature value that must be used in the effective absorption coefficient calculation.

The difficulty for selecting a suitable value of Θ to be adopted for a Ge crystal, was previously pointed out by Bröcker(12) in 1966. In consequence of the difference between the existing values of Θ for Ge, this author assumed the Debye Waller factor equal to unity, as an approximation to take into account the effect of the thermal motion of the atoms in a Ge neutron crystal monochromator. Hence, the Debye Waller factor can be calculated using the Debye temperature $\Theta = 370^{o}K$ chosen in the present work for Ge.

In figure 2 the results of eq.(10) are plotted, and the

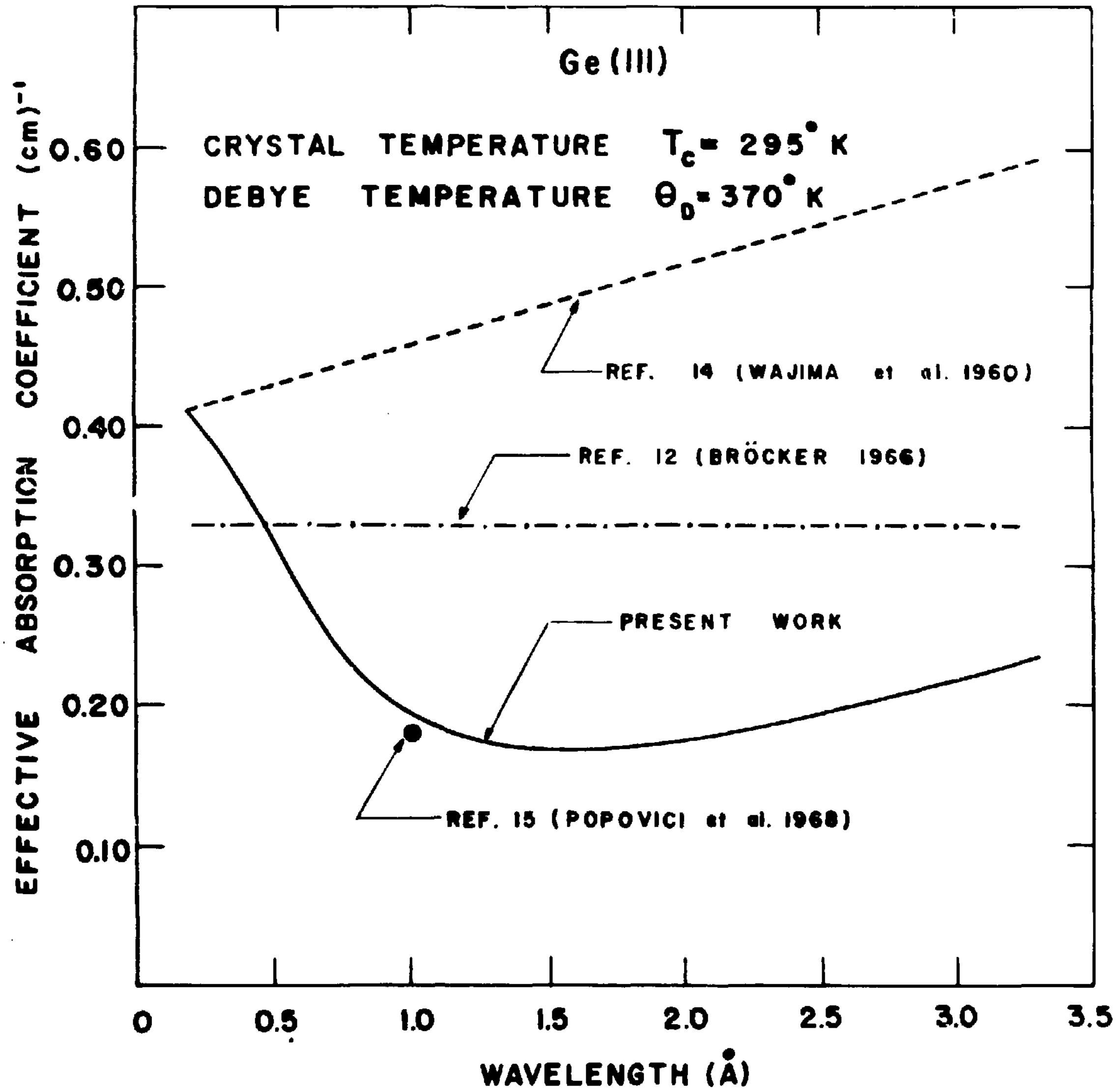

FIGURE 2.— Effective absorption coefficient of Germanium single crystal in Placzek incoherent approximation.

effective absorption coefficient for a Ge single crystal is showed over the wavelength range 0.1 to 3.5 Å (8.2 to 0.001 eV). For this calculation, the following values were used: T = 295°K, m = 12.049 x 10^{-23} g and 4.44 x 10^{22} atoms/cm^3. The values of the nuclear cross section are tabulated(13) and a program to perform calculation of the function $\Lambda(Z)$ was written for the IEA (IBM-1620) computer.

Calculations that involve the effective absorption coef ficient of the Ge crystal were previously made by other investigators(12,14). However, the total microscopic cross section of the element instead of the crystal was used. Wajima et al.(14) used $\mu = N (\sigma_a + \sigma_s)$ and Bröcker used a constant value $\mu = 0.33\ cm^{-1}$. In fact, only Popovici(15) in 1968 calculated the Ge crystal effective absorption coefficient, but only for the wavelength $\lambda = 1.0$ Å and his obtained value $\mu = 0.18\ cm^{-1}$ agrees with the present work result in this same wavelength.

III - CONCLUSIONS

With the measurements and calculations carried out in this work, the neutron energy dependence of the effective absorption coefficient for the Ge single crystal has been obtained. This result can be used in a calculation of the (111) planes reflectivity of this Ge crystal monochromator, as a function of the neutron energy.

The chosen Debye temperature value $\Theta = 370^{o}K$ can be useful in any calculation that involves neutrons and a Ge single crystal, in the energy range studied.

IV - ACKNOWLEDGEMENTS

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RESUMO

A secção de choque total para nêutrons de um monocristal de Germânio foi medida, usando o espectrômetro de cristal do IEA, para nêutrons com energias entre 1.0 e 0.01 eV, com o feixe incidindo perpendicularmente aos planos (111).

O comportamento em energia do coeficiente de absorção efetivo do cristal de Ge(111) foi obtido através de uma comparação entre as curvas calculadas da secção de choque total e os resultados experimentais.

O valor $\Theta = 370^{o}K$ para a temperatura de Debye do Ge foi escolhido entre os vários valôres existentes para o Ge.

RÉSUMÉ

En employant le spectromètre à cristal de l'IEA, la section efficace totale d'un mono-cristal de Germanium a été mesurée pour les neutrons d'énergies entre 1.0 et 0.01 eV, avec le faisceau incident qui arrive sur les plans (111) perpendiculairement.

Le comportement, en fonction de l'énergie du coefficient d'absortion effectif du Ge(111), a été obtenu après une comparaison des courbes calculées de section efficace totale et les résultats expérimentaux.

La valeur $\Theta = 370^{o}K$ pour la temperature de Debye a été choisie d'entre les differentes valeurs qui existent pour le Ge.

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