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RESUMO

No presente trabalho, os autores apresentam o cálculo da função resolução de um espectrômetro de cristal para nêutrons, em operação num dos canais experimentais do reator ... IEAR-1, bem como o cálculo da contaminação devida a nêutrons de segunda ordem para os planos (111) de um cristal de alumínio.

Para avaliar a influência dêsses efeitos nas medidas das secções de choque total para neutrons foi considerada a ressonância do irídio na energia E_o = 0,654 eV.

A curva teórica da ressonância foi calculada pela fórmula de Breit-Wigner levando em conta o alargamento de Doppler para a temperatura ambiente. Esta curva foi afetada pela função resolução e calculou-se a contaminação de neutrons de segunda ordem, obtendo-se a curva final que deve ser observada com o espectrômetro.

A ressonância foi medida pelo método da transmissão e os pontos experimentais concordam com a curva teórica esperada, indicando uma boa interpretação teórica dos efeitos considerados e uma precisa calibração do aparêlho.

RÉSUMÉ

On présente le calcul de la fonction resolution d'un spectromètre à cristal en opération à la sortie d'un tube d'irradiation du reacteur IEAR-1 et aussi le calcul de la contamination de neutrons de deuxième ordre pour les plans (111) d'un cristal d'aluminium.

Pour évaluer l'influence de ces effets sur les mesures des sections efficaces totales pour les neutrons, on a considéré la résonance de l'iridium dans l'énergie E_o = 0,654 eV.

La courbe théorique de la résonance a été calculée par la formule de Breit-Wigner, en prennant compte de l'élargissement Doppler à la température ambiante. Cette courbe a été affectée par la fonction résolution et on a calculé la contamination des neutrons de deuxiè-

me ordre, en obtenant ainsi une courbe finale a être mesurée.

La résonance a été mesuré par la méthode de transmission et les points expérimentaux sont en accord avec la courbe théorique espérée, ce qui indique une bonne interprétation théorique des effets considérés et une calibration precise de l'appareil.

ABSTRACT

The calculation of the resolution function of a neutron crystal spectrometer in operation at a beam hole of the IEAR-1 reactor is presented, as well as the calculation of the second order neutron contamination for the (111) planes of an aluminium crystal.

In order to estimate the influence of these effects in the neutron total cross section measurements, the iridium resonance at energy E_o = 0.654 eV, was considered.

The theoretical curve of the resonance was calculated using the Breit-Wigner formula, taking into account the Doppler broadening at room temperature. This curve was affected by the resolution function; the second order neutron contamination was calculated, and a final curve was obtained whose shape showed coincide with the experimental one.

The resonance curve was measured by the transmission method and the experimental points do agree with the expected theoretical curve, thus indicating a good theoretical interpretation of the considered effects and an accurate calibration of the instruments.

I. INTRODUCTION

The moderation of fission neutrons to thermal energies is one of the fundamental processes that must be considered in reactor design. During this slowing down process it is possible that neutron absorption takes place in capture resonances.

The measured shape of a resonance differs from its natural shape because of the effects of Doppler broadening. The Doppler effect results from the thermal motion of target nuclei , causing an effective increase in the width of the resonance as well as a change in the shape. Since the Doppler effect makes the resonance absorption cross section a function of temperature, the phenomenon

of Doppler broadening is of particular importance in reactor technology.

Having in mind a Doppler broadening study with variation of the sample temperature, a program of neutron resonance measurements near 1 eV was established.

This present work is a preliminary study where, using a crystal spectrometer, the effects that influence the neutron resonance measurement are estimated.

The effects considered here are: the instrumental resolution, the thermal motion of the atoms in the target, and the higher-order contamination in the reflected beam.

In order to estimate these effects, the neutron resonance of Ir at energy E_o = 0.654 eV was chosen, for two reasons: firstly because the level has a narrow width, and secondly because the sample exhibits a high purity (99,99%), which gives a good accuracy in the neutron total cross sections measurements.

II. EXPERIMENTAL METHOD

The source of neutrons for this work was the Instituto de Energia Atômica swimming pool research reactor operated at 2 MW. A crystal spectrometer, constructed at the IEA workshop, was used as monochromator.

In a general way, the spectrometer is similar to what has been described in the literature[1,2,3,4]. Angles may be read on a vernier scale with a precision of 0.01 degree. The supporting base of the crystal has six degrees of freedom and may be adjusted manually to optimize the alignment.

The instrument was located close to reactor core in a radial beam tube. The thermal neutron flux, measured with gold foils, outside the radial port, is 4×10^6 neutrons/cm^2.sec.

The collimator arrangement is shown schematically in figure 1, the first collimator in the incident beam and the second in the Bragg reflected beam, having angular divergence $a_1 = .2270^o$ and $a_2 = .2454^o$, respectively; both are of the "Soller" type.

In the measurements described in this paper, the (111) planes of an aluminium crystal were used for transmission monochromatization with mosaic $b = .159^o$, experimentally determined[5], and interplanar distance $d_{111} = 2{,}333$ Å.

The neutron detector is a BF_3 proportional counter 1 inch in diameter and 20 inches in length. It is filled to a pressure of 60 cm Hg with BF_3 enriched in B^{10} to 96 percent.

The efficiency of the detector can be calculated at any energy by the formula

$$\varepsilon = 1 - \exp\left[- N \times C \, E^{-1/2} \right] \qquad (1)$$

where N is the number of atoms per cm^3 in the counter, x is the counter length, C is the numerical constant that gives the 1/v slope of the B^{10} (n,α) Li^7 cross section, and E is the energy. For this particular counter the values of the constants are $N = 2.04 \times 10^{19}$ cm^{-3} and measurements of Sutton et al[6] give $C = 592 \times 10^{-24}$ for boron enriched to 96 percent in B^{10}.

An iridium powder sample, with $N = 3.97 \times 10^{-4}$ atoms/ /barn, was placed in an aluminium container and introduced into the beam in a reproducible position. The transmission through the sample was obtained by measuring the counting rate with the sample in the beam, and the rate obtained with an identical empty sample holder in the beam. The background was subtracted from each counting. The containers were designed to give a transmission which minimized the time required to reduce the statistical errors[7].

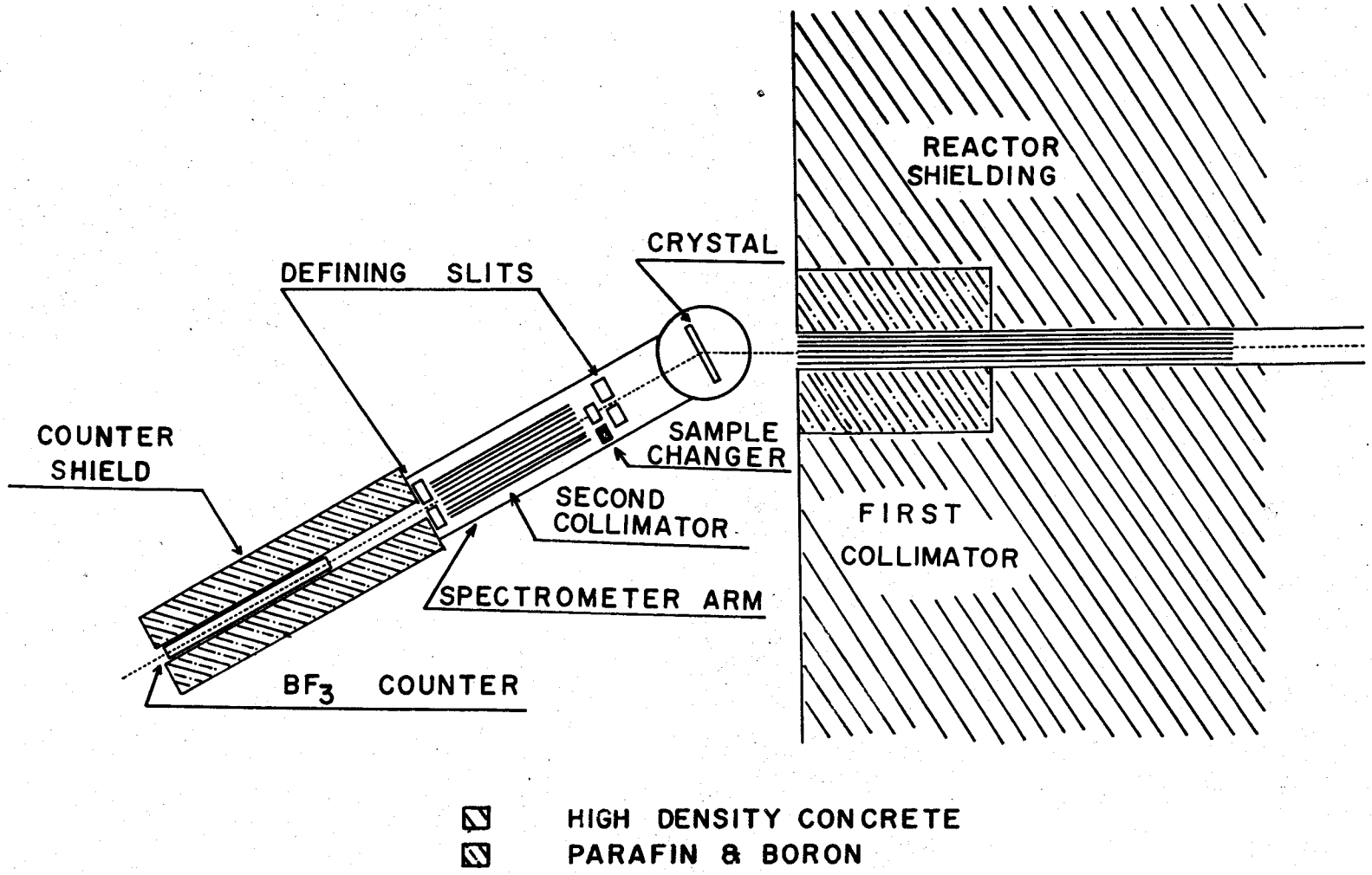

Figure 1 - Schematic diagram of the IEA neutron crystal spectrometer

To avoid the influence on the transmission of the fluctuations of the reactor power, the transmission measurements were repeated several times in cycles, according to a routine designed to cancel linear drifts.

The total cross sections were calculated from the transmission measurements. The conventional formula[7] has been used for the errors. The calculations were made by the IEA IBM-1620 computer.

III. THEORETICAL CALCULATION OF THE EFFECTS THAT INFLUENCE THE NEUTRON RESONANCE MEASUREMENT

A. THE CROSS SECTION BEFORE BROADENING

Each resonance represents an excitation state of the compound nucleus formed after the addition of a neutron to a capturing nucleus.

The total neutron cross section of an element presenting an isolated resonance having negligible resonant scattering can be expressed in terms of the one-level Breit-Wigner formula ,

$$\sigma_T = \sigma_o \Gamma^2 (E_o/E)^{1/2} \left[4(E - E_o)^2 + \Gamma^2\right]^{-1} + \sigma_{fa} \qquad (2)$$

where σ_T is the total cross section at energy E, σ_{fa} is the free atom scattering cross section, σ_o is the cross section exactly at the resonance E_o, and Γ is the total width of the resonance at half-maximum.

The parameter σ_o is actually a quantity involving the more fundamental parameters as follows:

$$\sigma_o = 4 \pi \lambda\!\!\!^{-2}_o \; f.g \; \Gamma_n \Gamma_\gamma / \Gamma^2$$

where $2 \pi \lambda\!\!\!^{-}_{o}$ is the neutron wavelength at resonance; g is the statistical weight factor that depends on the spin of the initial nucleus; $\Gamma_n = \Gamma_n^o \sqrt{E}$ and Γ_γ, are, respectively, the neutron and radiation widths.

Iridium has two resonances near 1 eV[8], the first at energy E_o = 0.654 eV is due to the isotope Ir^{191}, the second at energy E_o = 1.303 eV is assigned to Ir^{193} isotope. The contribution of each level to the total neutron cross section was calculated using Eq (2).

The contribution 1/v from far-away resonances of both isotopes was considered, calculating from

$$\sigma_{1/v} = \frac{g\,(0.286)^2 \times 10^{-16}}{4\,\pi\,\sqrt{E}} \cdot \sum_r \frac{f\,\Gamma_n^o\,\Gamma_\gamma}{E_r^2} \qquad (3)$$

This equation came from the capture term of the Breit--Wigner one level formula, making an approximation for E_o much bigger than E and Γ.

The total neutron cross section curve for the first resonance of iridium at E_o = 0.654 eV was constructed by adding contributions from all resonances appearing in the target material; previously published[9] parameters were used for this calculation, and the resulting curve, A, is shown in figure 2.

B. DOPPLER BROADENING

1B. Usual Form of the Doppler Broadening

The cross section formulae given in the previous section must now be modified to allow for the thermal motion of the target nuclei. The first ones that called attention to the Doppler effect in the case of neutron resonances were Bethe and Placzek[10] in 1937, treating the atoms as an ideal gas.

The cross section for non-stationary atoms for a given neutron energy is obtained by averaging the primitive cross section over the thermal distribution of velocities of the target nuclei.

The cross section that would result as a convolution of the natural line-shape with the Maxwellian Distribution of velocities was calculated.

The resulting expression for the effect is[11]

$$\sigma = \frac{\sigma_o}{\sqrt{\pi}\,\Delta}\sqrt{\frac{E_o}{E}}\int_o^\infty \frac{\exp\left[-\frac{(E_r - E_o)^2}{\Delta^2}\right]}{\left(\frac{E_r - E_o}{\Gamma/2}\right)^2 + 1}\, d E_r \qquad (4)$$

For a free gas the Doppler width Δ is given by

$$\Delta = 2(m E_o k T/M)^{1/2} \qquad (5)$$

where m and M are the masses of the neutron and of the nucleus, respectively, k the gas constant, and T the sample temperature.

E_r is the energy that correspond to V_r, the velocity of the incident neutron relative to the target nucleus.

Introducing non-dimensional variables such as

$$x = \frac{2\,(E - E_o)}{\Gamma}$$

$$y = \frac{2\,(E_r - E_o)}{\Gamma}$$

and

$$t = \left(\frac{\Delta}{\Gamma}\right)^2 ,$$

Eq (4) becomes

$$\sigma(E, \Psi) = \sigma_o \sqrt{\frac{E_o}{E}}\ \Psi(x,t) \qquad (6)$$

where $\Psi(x,t)$ is what we shall call the Doppler integral

$$\Psi(x,t) = \frac{1}{2\sqrt{\pi t}} \int_{-\infty}^{+\infty} \frac{\exp - \frac{(x-y)^2}{4t}}{1 + y^2}\, dy \qquad (7)$$

2B. Doppler Broadening for a Solid Absorber

The theory of neutron capture by atoms bound in a crystal was first considered in 1939 by Lamb[12]. In his theory Lamb considered the effects of lattice binding on the shape of a pure capture resonance.

Applying the methods of quantum mechanics, Lamb considered the Doppler distortion for a solid absorber assuming two limiting cases of lattice binding types: the strong and the weak binding approximation.

For the case of a strong binding Lamb finds that the resonance shape has no Doppler broadening.

In the weak binding assumption the shape of the broadened line for a solid absorber is the same as for the ideal absorber given by Eq (6). However, a new definition of Δ must be introduced: for the weak binding crystal, Δ depends on the average per degree of vibration and not on the sample's temperature as given in Eq (5).

Applying the Debye model, Lamb was able to establish a relationship between the average energy per degree of vibration of the crystal and the effective temperature T', which is to be used in the place of T.

Therefore, knowing the Debye temperature of a material one is able to determine the sample's effective temperature by the following relation[13].

$$\frac{T'}{T} = \frac{C_v}{24} + \frac{3\,(\theta/T)}{4\left[\exp\,(\theta/T) - 1\right]} + \frac{3\,(\theta/T)}{8} \qquad (8)$$

where $C_v = f(\theta/T)$ is the atomic heat function[14].

For iridium $T' \tilde{=} 1.04\ T$.

When the solid absorber is treated as a Debye crystal in the weak binding limit, Lamb has shown that the requirement

$$\Gamma + \Delta >> 2\theta \qquad (9)$$

must be satisfied.

Here Γ is the natural width of the resonance as previously defined, Δ is the effective Doppler width for the crystal, and θ is the sample's Debye temperature expressed in energy units. Egelstaff[15] has investigated this requirement in more detail, and his results indicate that the ratio $\frac{\Gamma + \Delta}{2\theta}$ needs only to be greater than approximately 2 before the weak binding model can be applied with confidence.

The required condition for the application of the effective temperature model, in the iridium resonance at 0.654 eV, is not rigorously satisfied. Nevertheless, the application of the theory of Lamb to account for the Doppler effect that it represents a good approximation for the theoretical Doppler broadened cross section.

For the iridium resonance at E = 0.654 eV the Doppler broadened cross section was calculated using Eq (6), being, also, added the 1/v contribution of the far-away resonances.

The resulting curve $\sigma(E, \Psi)$ is shown in curve B, in

figure 2.

C. EFFECT OF INSTRUMENTAL RESOLUTION

If the neutron beam were purely monoenergetic with an energy E, the value of the total cross section obtained from the measurements would be exactly the total Doppler broadened cross section $\sigma(E,\Psi)$.

For this ideal situation the transmission, T, through the sample is given by

$$T(E, \Psi) = \exp \left[- N \sigma (E, \Psi) \right] \tag{10}$$

where N is the number of target atoms per cm^2.

In practice, however, it is not possible to achieve this condition of a monoenergetic beam, and the instrumental resolution will cause the measured transmission T_R to differ from the true transmission $T(E, \Psi)$ as follows:

$$T_R = \frac{\int_o^\infty T (E,\Psi) R (E' - E) dE'}{\int_o^\infty R (E' - E) dE'} \tag{11}$$

where

$$R(E' - E) = A (E')^{-3.2} \exp - \left[\frac{4 \ln 2}{(\Delta E)^2} (E' - E)^2 \right] . \tag{12}$$

Eq (12) represents the spectrometer resolution function that gives the distribution in energy of the reflected neutron beam. The term $(E')^{-3.2}$ accounts for the reactor spectral distribution, the crystal reflectivity, and the 1/v variation of the detector efficiency; A is a numerical constant which will cancel in the normalization performed in Eq (11).

The nominal energy setting of spectrometer is E, and E' is the variable energy at which R is evaluated. The width of the resolution function at half-maximum is ΔE, and its value is given by

$$\Delta E = 4\, d \cos\theta\, (0.286)^{-1}\, E^{3/2}\, \Delta\theta \qquad (13)$$

if E is expressed in eV and d is 10^{-8} cm units.

$\Delta\theta$ is given by

$$\Delta\theta = \left(\frac{a_1^2 b^2 + a_1^2 a_2^2 + a_2^2 b^2}{a_1^2 + a_2^2 + 4b^2} \right)^{1/2} \qquad (14)$$

and represents the full width at half maximum of the instrument resolution function in terms of distribution in Bragg angle, i.e.,

$$J(\delta) = I\, K \exp\left[- \frac{4 \ln 2\, \delta^2}{(\Delta\theta)^2} \right] \qquad (15)$$

where I is the intensity and K is a numerical constant.

A detailed calculation of the function R(E'- E) and $J(\delta)$ can be found in Appendix A.

When the collimators and the crystal are chosen, the values of a_1, a_2 and b are fixed; then the value of $\Delta\theta$ in Eq(14) is a constant and a characteristic of the instrument.

For the IEA crystal spectrometer, where the collimators have angular divergence $a_1 = .2270^\circ$ and $a_2 = .2454^\circ$ respectively, and the aluminium crystal has the mosaic $b = .1590^\circ$, the value of $\Delta\theta$ therefore is $\Delta\theta = .1670^\circ \simeq 10'$.

From Eq(13) we can determine the resolution R at energy E.

We have

$$R = \frac{\Delta E}{E} = 2\, \Delta\theta\, \cot\theta$$

For the collimators and the Al crystal used in this experiment

$$R \simeq 7\% \text{ at } 0.5 \text{ eV}.$$

Eq(12) for $R(E' - E)$ may be inserted in Eq(11) giving the transmission T_R; the calculation for Eq(11) was made by the IEA IBM-1620 Computer.

The total cross section σ_R, that corresponds to T_R, was calculated for our iridium sample (with $N = 3.97 \times 10^{-4}$ atoms/barn) using the equation

$$\sigma_R = \frac{\ln T_R^{-1}}{N}$$

The curve C, shown in figure 2, represents σ_R.

D. HIGHER ORDER NEUTRON BEAM CONTAMINATION

The higher order contamination in the reflected beam is another effect that influences the neutron resonance measurement, and must be considered.

When a neutron energy is selected by Bragg's law

$$n\lambda = 2 d \sin \theta \qquad (16)$$

the reflected beam contains neutrons of energy E, 4E, 9E, etc , corresponding, respectively, to n = 1, 2, 3 etc; however, the primary energy E is the only one that interests in transmission measurements.

The knowledge of the spectral distribution allows the calculation of the higher-order contamination in the reflected beam. It is found in most cases that every order, except the second, can be neglected.

The relative intensity between second and first orders is given by the ratio[4]

$$k = \frac{I_2}{I_1} = \frac{(\varepsilon \, \Phi \, R \, \Delta E \, F)_2}{(\varepsilon \, \Phi \, R \, \Delta E \, F)_1} \qquad (17)$$

where the subscripts refer to the order.

Equation (17) may be simplified by using the information contained in the Appendix A where the coefficient of Eq (12) is evaluated.

$$\frac{(\varepsilon \, \Phi \, R)_2}{(\varepsilon \, \Phi \, R)_1} = \frac{\varepsilon_2}{\varepsilon_1} \left(\frac{E_2}{E_1} \right)^{-2.7}$$

The energy dependence upon the detector efficiency, in this case, is not approximated for 1/v, because the cross section changes sensibly for a small variation of k. The detector efficiency is given by Eq(1).

Besides this, returning to Eq(13)

$$\Delta E = \frac{4 \, d \, \cos \theta \, E^{3/2}}{(.286)} \, \Delta\theta$$

$$\frac{\Delta E}{E} = \frac{4d}{\lambda} \cos \theta \, \Delta\theta = 2 \frac{\cos \theta}{\operatorname{sen} \theta} \Delta\theta$$

$$\frac{\Delta E}{E} = 2 \, \Delta\theta \, \operatorname{cotg} \theta \cong 2 \frac{\Delta\theta}{\theta}$$

When comparing orders $\frac{\Delta\theta}{\theta}$ is constant, so

$$\frac{\Delta E_2}{\Delta E_1} = \frac{E_2}{E_1}$$

Then, Eq(17) becomes

$$k = \frac{I_2}{I_1} = \frac{\varepsilon_2}{\varepsilon_1} \left(\frac{E_2}{E_1} \right)^{-1.7} \frac{F_2}{F_1} \qquad (17a)$$

The term F does not depend on the energy but does depend on the order. It is defined as $F = e^{-2M}$, where f is the crystal structure factor, and e^{-2M} is the Debye-Waller temperature factor[16].

It is readily shown that for any order n, $M = n^2 M_1$. Details for computing M_1 can be found in ref. 16.

The ratio of the crystal structure factor for the first and second orders is $\frac{f_2}{f_1} = 1$ for the (111) planes of an aluminium crystal.

Then, Eq(17a) becomes

$$k = \frac{\varepsilon_2}{\varepsilon_1} \left(\frac{E_2}{E_1} \right)^{-1.7} e^{-6M_1} \qquad (18)$$

The Debye temperature of Al is $\Theta = 418^{\circ}$ K; therefore if the crystal is used at room temperature (295°K) the value of M_1 is 0.0414. Numerical substitution in Eq(18) gives the result

$$k = \frac{\varepsilon_2}{\varepsilon_1} (4)^{-1.7} e^{-0.2484} \qquad (18a)$$

The total cross section at each energy is obtained by measuring the sample transmission, and this value can be computed from the relationship

$$\frac{I}{i} = e^{N\sigma_m} \quad , \qquad (19)$$

where I is the intensity of the incident beam in the sample,

$$I = I_1 + I_2$$

being I_1 and I_2 the intensities for first and second order, respectively.

Similarly, for the transmitted intensity through the sample

$$i = i_1 + i_2 .$$

If the incident neutron beam were composed only of the first order neutrons, the measured cross section would be the σ_R from the preceding section, i.e., curve C in figure 2

$$\frac{I_1}{i_1} = e^{N\sigma_R} \tag{20}$$

Similarly, for the second order neutron beam

$$\frac{I_2}{i_2} = e^{N\sigma_2} \tag{21}$$

where σ_2 is the cross section at energy 4E.

Eq(20) and Eq(21) give

$$\frac{I_1}{I_2}\,\frac{i_2}{i_1} = e^{N(\sigma_R - \sigma_2)} \quad ;$$

being $k = \frac{I_2}{I_1}$, we have

$$\frac{i_2}{i_1} = k\, e^{N(\sigma_R - \sigma_2)} \quad ;$$

$$e^{N\sigma_m} = \frac{I_1 + I_2}{i_1 + i_2} = \frac{I_1\,(1 + \frac{I_2}{I_1})}{i_1\,(1 + \frac{i_2}{i_1})}$$

$$e^{N\sigma_m} = e^{N\sigma_R}\left[\frac{1 + k}{1 + k \exp N\,(\sigma_R - \sigma_2)}\right]$$

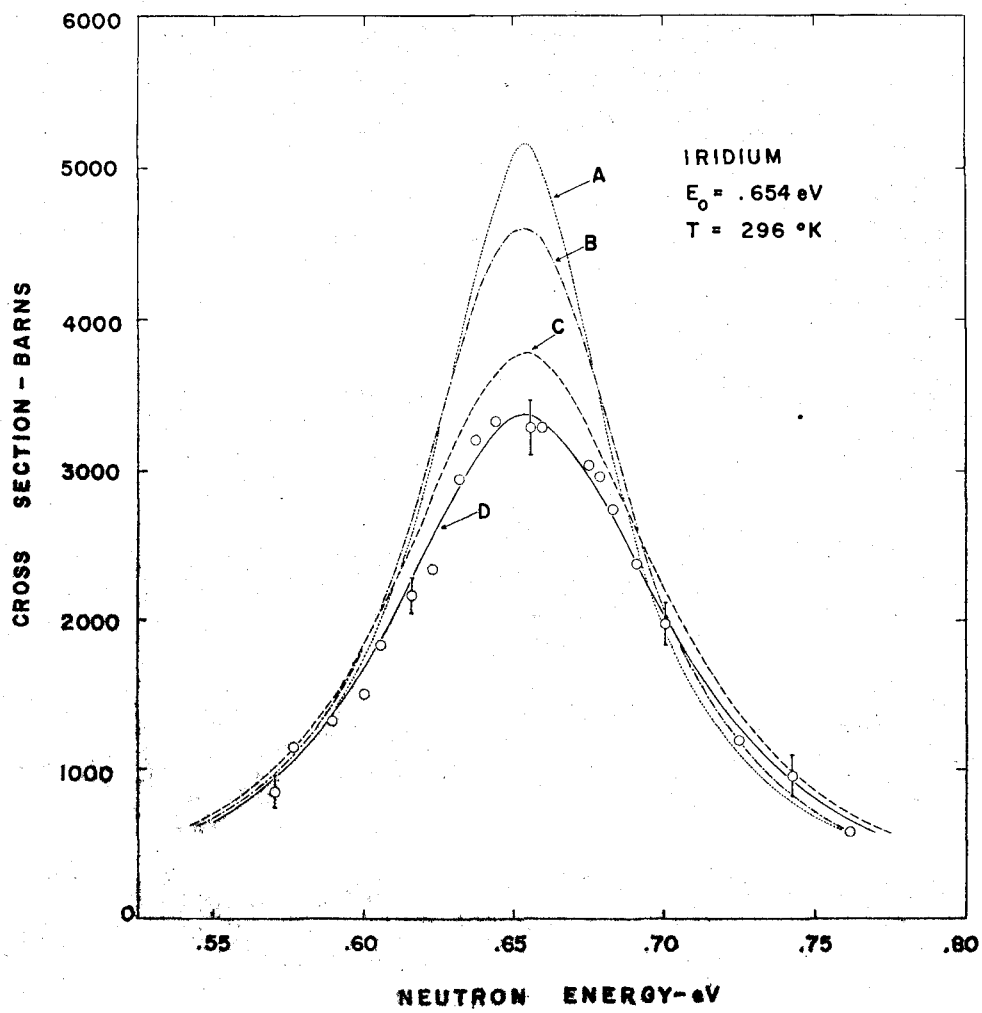

Figure 2 - Total cross section of iridium as a function of energy at room temperature. Curve A is the theoretical Breit-Wigner shape. Curve B results from operating on A with Doppler broadening according to the effective temperature model. Curve C is obtained by operating on B with the resolution function of the spectrometer. Curve D is obtained by operating in C with the second order neutron contamination from the (111) planes of a Al crystal.

$$\sigma_m = \sigma_R + \frac{1}{N} \ln \left[\frac{1 + k}{1 + k \exp N (\sigma_R - \sigma_2)} \right] \qquad (22)$$

The range of the primary energy in the case of the iridium resonance measurement at 0.654 eV, makes it possible to take $\sigma_2 \tilde{=} 25$ barns[9] for the cross section in 4E energy.

The latter Eq(22) corresponds to the Breit-Wigner natural line shape, as affected by the Doppler effect, the instrumental resolution and the second order contamination.

The cross section σ_m is the theoretical value that must be measured; it is represented in curve D of figure 2.

IV. EXPERIMENTAL DATA AND CONCLUSIONS

The total neutron cross section for iridium was measured in the energy range of 0.55 eV to 0.8 eV; a reasonable agreement between the experimental points and the theoretical curve D in figure 2 was found.

It is not possible to verify all the effects considered in this paper by any direct experimental measurement; however, the experimental results indicate a good estimative for the resolution function, the second order contamination and the used parameters.

The collimator arrangement and the crystal used in the IEA crystal spectrometer, for this experiment, is not ideal for providing a monochromator system of good intensity and resolution; however, this system is good enough for estimating the already mentioned effects.

In order to develop accurate Doppler broadening measurements in neutron resonances, the spectrometer resolution must be improved. Having this aim in mind, collimators with smaller angular divergences and crystals with narrower mosaic structure are being

designed and sought, so that $\Delta\theta$, which defines the resolution, in Eq(14), will become smaller.

A technique for the elimination of the second order neutron contamination in the beam was developed by use of a tellurium filter. Tellurium has been chosen because it is pratically transparent for neutrons having an energy lower than 1 eV and because it absorbs neutrons in the region near 2.5 eV, which is the energy range of second order neutrons having an energy 4E.

With this technique we succeeded in eliminating the second order effect in the iridium resonance at $E_o = 0.654$ eV ; thus the measured cross sections are coincident with the curve σ_R in curve C of figure 2.

We are now developing the optimization of the filter's thickness; the obtained results will be published in a later paper.

The elimination of higher order effects constitutes another confirmation of the good interpretation of the effects that influence the measurement of a resonance, presented in this paper.

APPENDIX A

IA. DERIVATION OF THE RESOLUTION FUNCTION: IN TERMS OF DISTRIBUTION IN BRAGG ANGLE

(case $a_1 \neq a_2 \neq b$)

It is possible to derive an approximation to the resolution function, from the geometrical arrangement of the spectrometer[17]. The experimental arrangement considered here is for two "Soller" collimators - the first one in the incident beam and the other one on the spectrometer arm.

Collimators: The intensity of the beam emerging from the first collimator, as approximated by a gaussian distribution, is given by[17]

$$I(\phi_1) = I_o \exp\left[-(\phi_1/\alpha_1)^2\right] \qquad (A.1)$$

where ϕ_1 is the angle between the individual incident ray and the central incident ray and

$$\alpha_1 = \frac{a_1}{2(\ln 2)^{1/2}} .$$

Similarly, for the second collimator

$$A(\phi_2) = \exp\left[-(\phi_2/\alpha_2)^2\right] , \qquad (A.2)$$

where A is normalized to unity.

The collimator divergence a is determined by the ratio of the width s to the length l of the individual collimator channels; i.e., $a = s/l$.

Crystal: The crystal considered as composed of mosaic blocks each

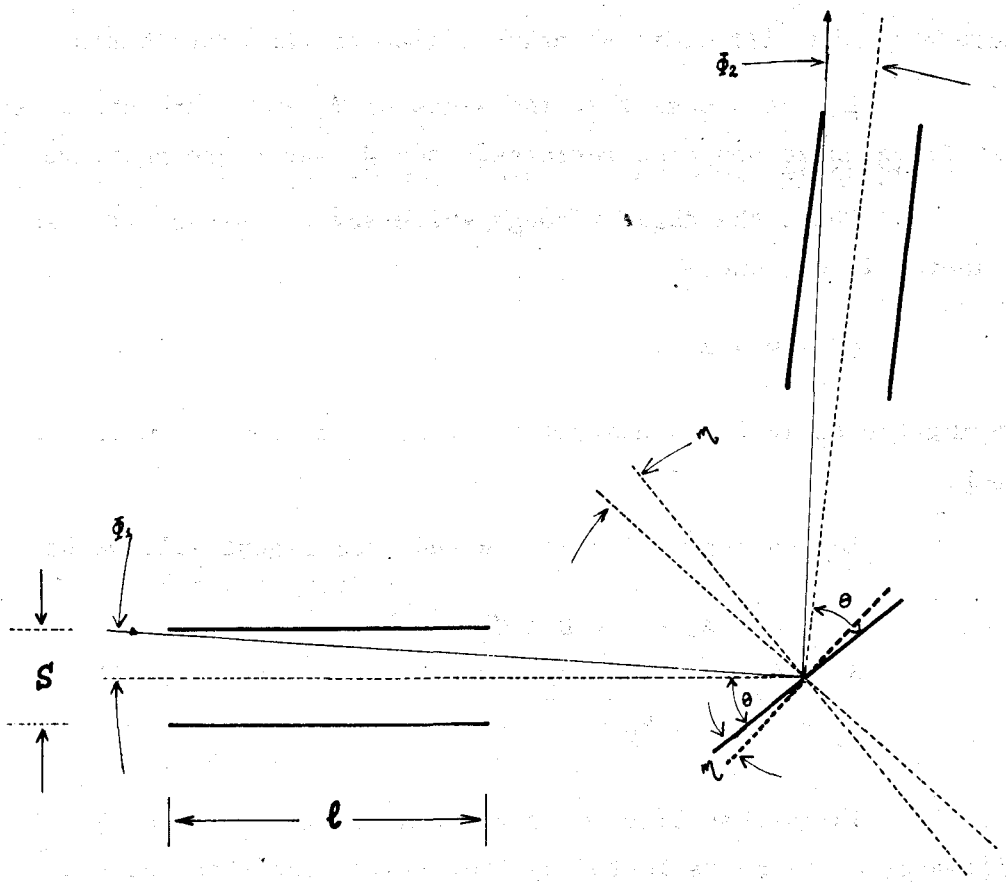

Figure A.1 - Schematic arrangement of neutron beam collimation

of them individually perfect, but oriented in a distribution about an average position[17]. Let us assume that the projections on the horizontal plane of the normals to any given set of crystal planes have a gaussian distribution, $\Theta(\eta)$, where

$$\Theta(\eta) = R_o(\beta) \exp \left[- (\eta/\beta)^2 \right] , \qquad (A.3)$$

where η is the angle between the individual mosaic block and the central mosaic block and

$$\beta = \frac{b}{2\ (\ln 2)^{1/2}} \ ,$$

where b is the full width at half-maximum of the distribution.

Let us assume that the signs of ϕ_1 and η are chosen so that Bragg angle would be increased when ϕ_1 and η are positive.

Thus, the angle through which any individual ray is reflected is θ', where

$$\theta' = \theta + \phi_1 + \eta \ , \qquad (A.4)$$

θ being the angle for a central ray reflected from a central mosaic block.

Let us define $\delta = \theta' - \theta$ and from figure A.1, we have

$$\begin{aligned} \theta' &= \theta + \phi_1 + \eta = \theta + \phi_2 - \eta \\ \delta &= \phi_1 + \eta \ ; \ \delta = \phi_2 - \eta \\ \theta_1 &= \delta - \eta \ ; \ \phi_2 = \delta + \eta \end{aligned} \qquad (A.5)$$

The probability for a neutron passing through the first collimator of being reflected by the crystal and then passing through the second collimator to the detector may be expressed as a function of δ

$$J(\delta) = \int_{\phi_1'^a}^{\phi_1'^b} I(\phi_1)\ \Theta\ (\eta)\ A(\phi_2)\ d\ \phi_1 \qquad (A.6)$$

Inserting Eqs(A.1-4) in Eq(A.6) and changing the variable to η we obtain

$$J(\delta) = I_o R_o \int_{\eta'^b}^{\eta'^a} d\eta \exp - \left[\left(\frac{\delta - \eta}{\alpha_1}\right)^2 + \left(\frac{\eta}{\beta}\right)^2 + \left(\frac{\delta + \eta}{\alpha_2}\right)^2 \right] . \qquad (A.7)$$

Taking only the exponent in Eq(A.7)

$$\frac{(\delta - \eta)^2}{\alpha_1^2} + \frac{\eta^2}{\beta^2} + \frac{(\delta + \eta)^2}{\alpha_2^2} = \frac{(\delta^2 - 2\delta\eta + \eta^2)}{\alpha_1^2} + \frac{\eta^2}{\beta^2} + \frac{(\delta^2 + 2\delta\eta + \eta^2)}{\alpha_2^2} =$$

$$= \frac{\alpha_2^2\beta^2\,(\delta^2 - 2\delta\eta + \eta^2) + \eta^2\,\alpha_1^2\,\alpha_2^2 + \alpha_1^2\,\beta^2\,(\delta^2 + 2\delta\eta + \eta^2)}{\alpha_1^2\,\beta^2\,\alpha_2^2} \quad ;$$

making

$$A = \alpha_2^2\beta^2 + \alpha_1^2\alpha_2^2 + \alpha_1^2\beta^2 \quad ,$$

$$2B = 2\beta^2\left[\alpha_1^2\delta - \alpha_2^2\delta\right] \quad , \qquad (A.8)$$

$$C = \beta^2\left[\alpha_1^2\delta^2 + \alpha_2^2\delta^2\right] \quad ,$$

and $$D = \alpha_1^2\beta^2\alpha_2^2 \quad ,$$

the integral becomes

$$\int_{-\infty}^{+\infty} d\eta \;\; \exp - \left[\frac{A\eta^2 + 2B\eta + C}{D}\right] = \int_{-\infty}^{+\infty} d\eta \;\; \exp - \left[\frac{\eta^2 + 2\,\frac{B}{A}\,\eta + \frac{C}{A}}{D/A}\right]$$

$$= \int_{-\infty}^{+\infty} d\eta \; \exp - \left[\frac{(\eta + \frac{B}{A})^2 + \frac{C}{A} - \frac{B^2}{A^2}}{D/A}\right] = e^{-\left[\frac{CA - B^2}{DA}\right]} \int_{-\infty}^{+\infty} d\eta \; e^{-\left[\frac{(\eta + \frac{B}{A})^2}{D/A}\right]^2}$$

Making

$$\eta + \frac{B}{A} = x \quad , \quad \frac{D}{A} = \frac{1}{a^2} \qquad \text{and}$$

dx = dy, the latter integral becomes

$$= 2\int_0^{\infty} e^{-a^2x^2}\, dx \;=\; 2.\,\frac{\sqrt{\pi}}{2a} = \sqrt{\frac{D\pi}{A}} \quad ;$$

the expression (A.7) becomes

$$J(\delta) = I_o R_o \sqrt{\frac{D\pi}{A}}\; e^{-\left[\frac{CA - B^2}{DA}\right]} \quad . \qquad (A.10)$$

Taking only the exponent and substituting the values given in (A.8) for A, B, C and D, we have

$$\frac{CA - B^2}{DA} = \frac{1}{DA}\left[\beta^2\delta^2(\alpha_1^2+\alpha_2^2)\right](\alpha_2^2\beta^2 + \alpha_1^2\alpha_2^2 + \alpha_1^2\beta^2) - \beta^4\delta^2(\alpha_1^2 - \alpha_2^2)^2 =$$

$$= \frac{\beta^2\delta^2}{DA}\left[(\alpha_1^2 + \alpha_2^2)\,(\alpha_2^2\beta^2 + \alpha_1^2\alpha_2^2 + \alpha_1^2\beta^2) - \beta^2(\alpha_1^2 - \alpha_2^2)^2\right] =$$

$$= \frac{\beta^2\delta^2}{DA}\,(\alpha_1^2\alpha_2^2\beta^2 + \alpha_1^4\alpha_2^2 + \alpha_1^4\beta^2 + \alpha_2^4\beta^2 + \alpha_1^2\alpha_2^2 + \alpha_1^2\alpha_2^2\beta^2 -$$

$$- \beta^2\alpha_1^4 + 2\beta^2\alpha_1^2\alpha_2^2 - \beta^2\alpha_2^4\,) =$$

$$= \frac{\delta^2}{DA}\,(\alpha_1^4\alpha_2^2\beta^2 + 4\alpha_1^2\alpha_2^2\beta^4 + \alpha_1^2\alpha_2^4\beta^2\,) =$$

$$= \frac{\delta^2}{A}\,\frac{(\alpha_1^4\alpha_2^2\beta^2 + 4\alpha_1^2\alpha_2^2\beta^4 + \alpha_1^2\alpha_2^4\beta^2)}{\alpha_1^2\alpha_2^2\beta^2} =$$

$$\delta^2 = \frac{(\alpha_1^2 + 4\beta^2 + \alpha_2^2\,)}{(\alpha_2^2\beta^2 + \alpha_1^2\alpha_2^2 + \alpha_1^2\beta^2)} \quad .$$

Going back to Eq(A.10) and taking the coefficient, we have

$$\frac{D\,\pi}{A} = \pi^{1/2}\,\left(\frac{\alpha_1^2\beta^2\alpha_2^2}{\alpha_2^2\beta^2 + \alpha_1^2\alpha_2^2 + \alpha_1^2\beta^2}\right)^{1/2} =$$

$$= \pi^{1/2} \left(\frac{1}{\frac{1}{\alpha_1^2} + \frac{1}{\alpha_2^2} + \frac{1}{\beta^2}} \right)^{1/2} .$$

Thus, Eq(A.10) becomes

$$J(\delta) = I_o R_o \pi^{1/2} \left(\frac{1}{\frac{1}{\alpha_1^2} + \frac{1}{\alpha_2^2} + \frac{1}{\beta^2}} \right)^{1/2} \exp - \left[\frac{(\alpha_1^2 + \alpha_2^2 + 4\beta^2)\ \delta^2}{(\alpha_2^2\beta^2 + \alpha_1^2\alpha_2^2 + \alpha_1^2\beta^2)} \right] \tag{A.11}$$

Substituting the expression for α_1, α_2 and β, we obtain

$$J(\delta) = IK \exp \left[- \frac{4 \ln 2\ \delta^2}{(\Delta\theta)^2} \right] . \tag{A.12}$$

This Eq(A.12) represents the instrument resolution function in terms of distribution in Bragg angle, where I is the intensity, K is a numerical constant and $\Delta\theta$ is the full width at half-maximum of the distribution $J(\delta)$.

$$\Delta\theta = \left(\frac{a_1^2 b^2 + a_1^2 a_2^2 + a_2^2 b^2}{a_1^2 + a_2^2 + 4b^2} \right)^{1/2} \tag{A.13}$$

II.A ENERGY DISTRIBUTION OF THE MONOCHROMATIC BEAM

Let us[16] now transform Eq(A.12) to a distribution in energy. The equation may be rewritten as

$$J(\delta) = IK \exp - \left[\frac{4 \ln 2\ (\theta' - \theta)^2}{(\Delta\theta)^2} \right] . \tag{A.12a}$$

Taking only the exponent in Eq(A.12a), we may have $\Delta\theta$ and $\delta = \theta' - \theta$ in terms of energy.

Bragg's law for the first-order reflection (n=1) is given by

$\lambda = 2\ d \sin\theta$, with $\lambda = CE^{-1/2}$, where $C = 0.286$.

Let us assume $\Delta\theta = f(E)$. From Bragg's law we have

$$\Delta\lambda = 2\ d \cos\theta\ \Delta\theta\ ,$$

$$\Delta\lambda = -\frac{C}{2}\ E^{-3/2}\ \Delta E\ , \quad \therefore$$

$$-\frac{C}{2}\ E^{-3/2}\ \Delta E = 2\ d \cos\theta\ \Delta\theta \quad \therefore$$

$$\Delta\theta = \frac{-\ C/2\ E^{-3/2}\ \Delta E}{2\ d\ \cos\theta}\ .$$

Now let us assume $\delta = f(E,E')$. We have

$$C(E')^{-1/2} = 2\ d \sin\theta'\ ,$$

$$C(E)^{1/2} = 2\ d \sin\theta\ ,$$

$$(E')^{-1/2} - (E)^{-1/2} = \frac{2d}{C}\ (\sin\theta' - \sin\theta)$$

with

$$(\sin\theta' - \sin\theta) = 2 \sin 1/2\ (\theta' - \theta) \cos 1/2\ (\theta' + \theta)$$

since

$(\theta' - \theta) \equiv \delta \leq 20$ minutes of arc, i.e., $\delta \leq 2\Delta\theta$ (twice the full width at half maximum of the distribution in Bragg angle given by Eq(A.12).

Thus, $2 \sin 1/2\ (\theta' - \theta) \tilde{=} (\theta' - \theta)$ and

$\cos 1/2\ (\theta' + \theta) \tilde{=} \cos\theta$; we get

$(\sin\theta' - \sin\theta) \tilde{=} (\theta' - \theta) \cos\theta$.

So, we obtain

$$(E')^{-1/2} - (E)^{-1/2} = \frac{2d}{C} (\theta' - \theta) \cos\theta \ ,$$

$$\delta \equiv (\theta' - \theta) = \frac{C \left[(E')^{-1/2} - (E)^{-1/2}\right]}{2\, d \cos\theta} \ .$$

Substituting $\Delta\theta$ and δ in the exponent of Eq(A.12a), we have

$$\exp - \left[\frac{16 \ln 2}{(\Delta E)^2} \ \frac{\left[(E')^{-1/2} - (E)^{-1/2}\right]^2}{E^{-3}} \right] .$$

But

$$E^3 \left[(E')^{-1/2} - (E)^{-1/2}\right]^2 = E^3 \left[\left(\frac{1}{E'}\right) - \frac{2}{(EE')^{1/2}} + \left(\frac{1}{E}\right) \right] =$$

$$= E^2 \left[\left(\frac{E}{E'}\right) - 2\left(\frac{E}{E'}\right)^{1/2} + 1 \right] = E \left[1 - \left(\frac{E}{E'}\right)^{1/2} \right]^2 .$$

A Taylor's expansion of $(E/E')^{1/2}$ about $E' = E$ gives $(E/E')^{1/2} = 1 - \frac{1}{2} \frac{1}{E} (E' - E) + \ldots$

All higher terms are negligible in our case.

Then, the exponent becomes

$$\left[\frac{4 \ln 2}{(\Delta E)^2} \ (E' - E)^2 \right] \qquad (A.14)$$

Let us considerer now the coefficient in Eq(A.12a).

The energy dependence of the observed neutron intensity distribution, may be expressed in the form[18]

$$I(E') = A \varepsilon \phi R \Delta E, \qquad (A.15)$$

where A is a numerical constant, ε is the detector efficiency, ϕ is the spectral distribution of the reactor, R is the reflectivity of the crystal, and ΔE is the resolution width of the spectrometer.

Since the expressions for ε and ΔE are known, the energy dependence of the product $\phi R = \frac{I}{\varepsilon \Delta E}$ can be determined. The intensity above 0.5 eV was measured and corrected for ε and ΔE; a least squares fit to the experimental values of $I/\varepsilon\Delta E$ gives $\phi R \; \alpha E'^{-2.7}$ (see figure A.2).

The energy dependence $I(E')\alpha(E')^{-3.2}$ is given by Eq(A.15) with $\phi R \; \alpha(E')^{-2.7}$ and $\varepsilon \; \alpha(E')^{-0.5}$.

Equation (A.12a) may be rewritten as

$$R(E' - E) = A(E')^{-3.2} \exp - \left[\frac{4 \ln 2}{(\Delta E)^2} (E' - E)^2 \right], \quad (A.16)$$

This Eq(A.16) represents the resolution function when the energy setting of the spectrometer is E. E' is the variable energy at which R is evaluated and A is a numerical constant. The width of the resolution function at half maximum is ΔE, and its value is given by

$$\Delta E = 4 \, d \cos \theta \, (0.286)^{-1} E^{3/2} \, \Delta\theta \qquad (A.17)$$

if E is expressed in eV and d in 10^{-8} cm units.

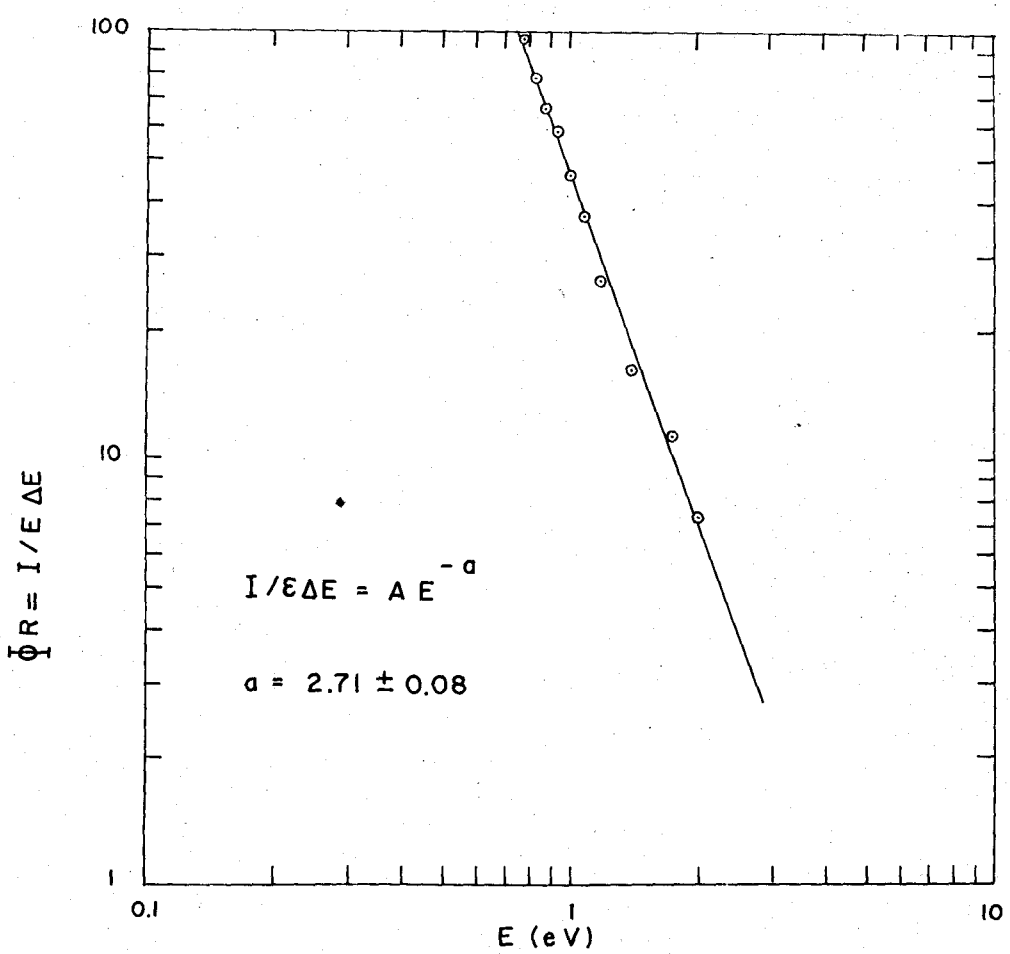

Figure A.2 - The neutron intensity I as a function of energy. The curve was corrected for detector efficiency ε and resolution width ΔE. The least squares fit shows that $\emptyset R \alpha E^{-2.7}$.

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