

from the present experiment agrees very well with the latest direct γ -energy determination of Kruger and Ogle¹⁰ which gave 1.70 ± 0.02 Mev. It is somewhat higher than the value 1.67 Mev which Wattenberg obtains from the mean energy of the photo-neutron source.

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Scattering of Neutrons in Polycrystals*

R. J. FINKELSTEIN**

Argonne National Laboratory, Chicago, Illinois

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Although elastic and first-order inelastic cross sections for a neutron against a Debye crystal have already been determined, expressions for higher order inelastic collisions have not been calculated, and would be very complex for the Debye model. The calculation of the total inelastic cross section involving the emission of an arbitrarily large number of phonons is here presented for a neutron against an Einstein polycrystal. The result, as one would expect, is essentially the same as that given by Fermi for amorphous scatterers, except at high neutron energies where we have calculated the cross section for the ejection of the struck nucleus from its lattice. The coherent elastic cross section is also determined; it is important for energies as high as 1 volt, and does not differ appreciably from that previously calculated for a Debye crystal. The total cross section, the sum of the coherent and incoherent parts, is compared with the experimental data on beryllium.

1. INTRODUCTION

THE scattering of a neutron by a crystal may be described qualitatively in the following manner. As long as its energy is large compared to the chemical binding energy of the lattice, the neutron is scattered as if the nuclei forming the lattice were free. A fast neutron therefore slows down by dislocating effectively free nuclei until its energy becomes of the order of the crystal bond. It then makes inelastic collisions with the lattice as a whole, until it loses so much more energy that its wave-length exceeds the amplitude of the temperature vibrations of the scattering nuclei. At this point elastic collisions with the lattice become the most probable process and further cooling of the neutron takes place very slowly. Finally, if the neutron energy is somehow made still lower, inelastic scattering becomes important again,

since the neutron begins to absorb energy from the crystal.

In this paper the cross sections for these different kinds of scattering are calculated for the Einstein crystal. The elastic and first-order inelastic cross sections have already been determined for the Debye crystal.¹ The difference between our formula for elastic scattering and that deduced from the Debye model is insignificant. For first order inelastic collisions the Debye type of formula is to be preferred, but for higher order collisions, in which many phonons are exchanged, the equations of the Debye model become too complex. In these higher order collisions the cross section computed from the Einstein model is essentially identical with the cross section calculated by Fermi² to describe

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** Now at the Institute for Advanced Study, Princeton, New Jersey.

¹ I. Pomerantschuk, *Physik. Zeits. d. Sowjetunion* **13**, 65 (1938); R. Weinstock, *Phys. Rev.* **65**, 1 (1944). See also Halpern, Hamermesh, and Johnson, *ibid.* **59**, 981 (1941); Wick, *Physik. Zeits.* **38**, 403 (1937); Seeger and Teller, *Phys. Rev.* **62**, 37 (1942).

² E. Fermi, *Ricerca Sci.* **7**, 13 (1936); H. A. Bethe, *Rev. Mo d. Phys.* **9**, 124 (1937).

the thermalization of neutrons in hydrogenous substances. The cross section is incoherent and the formula for it is hence applicable to amorphous matter. In the same energy interval in which higher order inelastic collisions become dominant, the elastic cross section, which is a discontinuous function of energy in the thermal region, becomes effectively continuous. Finally, at still higher neutron energies the Einstein model of the crystal must be modified because the nucleus struck by the neutron may be ejected from the lattice.

Before describing the calculations, we distinguish between two ways of regarding a crystal as a set of equivalent oscillators. (a) The nuclei comprising the crystal may be considered as independent oscillators whose frequencies are all equal. In this picture an inelastic collision in which many phonons are absorbed or emitted by the lattice occurs when a single oscillator makes a *many-quantum* transition. (b) The motions of the individual nuclei may be analyzed into $3N$ lattice vibrations whose frequencies are all equal. In this picture a collision involving many phonons is described as a combination of simultaneous *one-quantum* transitions of many lattice vibrations. Description (b) is easier to connect with the Debye model, whereas description (a), which we use here, can be reduced to the problem of scattering by a single isotropic oscillator.

2. THE MATRIX ELEMENTS

The wave function for a composite system consisting of a crystal and a free neutron is

$$\psi(\mathbf{k}, \mathbf{n}_1 \cdots \mathbf{n}_N) = \exp(i\mathbf{k} \cdot \mathbf{r}) \prod_1^N \varphi(\mathbf{u}_j, \mathbf{n}_j). \quad (1)$$

In Eq. (1), \mathbf{k} and \mathbf{r} are wave number and position vectors of the neutron; \mathbf{u}_j is the displacement of the j th oscillator from its equilibrium position, and \mathbf{n}_j is the set of three quantum numbers needed to describe this oscillator. The functions, φ , are products of Hermite functions. We calculate the matrix element for a transition in which the neutron changes from state \mathbf{k} to \mathbf{k}' while the crystal simultaneously makes a transition from $(\mathbf{n}_1 \cdots \mathbf{n}_N)$ to $(\mathbf{n}_1' \cdots \mathbf{n}_N')$ as a result of the following interaction potential² between the neutron

and the crystal:

$$V = \sum_1^N A_j \delta(\mathbf{r} - \mathbf{r}_j) \quad (2)$$

where \mathbf{r}_j is the instantaneous position of the j th nucleus. The evaluation of this matrix element depends on whether the collision is elastic or inelastic. The results are

$$\begin{aligned} & (\mathbf{k}, \mathbf{n}_1 \cdots \mathbf{n}_N | V | \mathbf{k}' \mathbf{n}_1 \cdots \mathbf{n}_N) \\ &= \sum_1^N A_j (\mathbf{n}_j | I | \mathbf{n}_j) \exp[i(\mathbf{k} - \mathbf{k}') \cdot \mathbf{R}_j] \end{aligned} \quad (3a)$$

for elastic collisions, and

$$\begin{aligned} & (\mathbf{k}, \mathbf{n}_1 \cdots \mathbf{n}_p \cdots \mathbf{n}_N | V | \mathbf{k}' \mathbf{n}_1 \cdots \mathbf{n}_p' \cdots \mathbf{n}_N) \\ &= A_p (\mathbf{n}_p | I | \mathbf{n}_p') \exp[i(\mathbf{k} - \mathbf{k}') \cdot \mathbf{R}_p] \end{aligned} \quad (3b)$$

for inelastic collisions. Here

$$\begin{aligned} (\mathbf{n}_j | I | \mathbf{n}_j') &= \int_{-\infty}^{+\infty} \exp[i(\mathbf{k} - \mathbf{k}') \cdot \mathbf{u}_j] \varphi(\mathbf{u}_j, \mathbf{n}_j) \\ &\quad \times \varphi(\mathbf{u}_j, \mathbf{n}_j')^* d\mathbf{u}_j \end{aligned} \quad (4)$$

and $\mathbf{R}_j (= \mathbf{r}_j - \mathbf{u}_j)$ is the equilibrium position of the j th nucleus. The probability of an elastic collision, being proportional to the square of the sum in (3a), contains cross terms which represent interference between neutron waves scattered from different oscillators; elastic scattering is therefore coherent. On the other hand, matrix elements describing inelastic collisions consist of single terms only, so that there is no interference; inelastic scattering by an Einstein crystal is hence incoherent and the scattering is isotropic. This feature of the present model is in error for *nearly* elastic scattering, which is not isotropic either according to the Debye model or to the experimental evidence on x-rays; but for larger energy transfers our simple model should be correct.

3. THE SCATTERING CROSS SECTION

In terms of the matrix element M_{AB} the cross section for a transition from state A to state B is, per unit solid angle,

$$\begin{aligned} \sigma_{AB} &= a |M_{AB}|^2 \\ a &= (4\pi^2 m_N^2 / Nh^4) (V' / V) \end{aligned}$$

where A and B refer to states of the composite

system consisting of the crystal and the neutron. The initial and final velocities of the neutron are V and V' , and its mass is m_N . The cross section is here normalized by dividing by the number, N , of nuclei in the crystal. If P_A is the probability that the crystal is in state A , then the total cross section is

$$\sigma = a \sum_{A,B} P_A |M_{AB}|^2. \quad (5)$$

The total elastic cross section σ^0 is obtained by carrying the sum (5) over only those final states for which $E_A = E_B$, where E is the energy of the indicated state of the crystal. Likewise the sum giving the total-absorption (emission) cross section, $\sigma^+(\sigma^-)$, is limited by the conditions $E_B > E_A$ and $E_B < E_A$, respectively; here emission (absorption) means emission (absorption) of phonons by the *neutron*.

If the matrix elements (3) are put in (5), one gets the scattering cross section of a monocrystal in terms of single oscillator functions. The results are, of course, quite different for the elastic and inelastic cases.

A. Inelastic Cross Section

The result for the inelastic case is

$$\sigma^\pm = (m_N/\mu)^2 \sigma_i J^\pm \quad (6)$$

where

$$J^\pm = \int I^\pm d\Omega \quad (6a)$$

is the integral of I^\pm over all solid angle, and

$$I^\pm = (1/4\pi) \sum (V'/V) P(\mathbf{n}) |\langle \mathbf{n} | I | \mathbf{n}' \rangle|^2. \quad (6b)$$

$P(\mathbf{n})$ is the probability that a single oscillator is in the state \mathbf{n} ; $\langle \mathbf{n} | I | \mathbf{n}' \rangle$ is given by (4). In Eq. (6) σ_i is the incoherent cross section of a unit cell, namely,

$$\sigma_i = (1/p) \sum' \sigma_p \quad (6c)$$

where the sum is to be carried over all p nuclei in a unit cell; σ_p is the cross section of a free nucleus.

$$\sigma_p = (16\pi^3 \mu^2 / h^4) A_p^2 \quad (6d)$$

where μ is the reduced mass of the neutron and free nucleus.

Since the inelastic scattering is incoherent, it is the same for the polycrystal as for the monocrystal.

B. Elastic Cross Section

The elastic cross section³ of a single crystal, also found by putting (3) in (5), is per unit solid angle

$$\sigma^0 = (m_N/\mu)^2 [(2\pi^2 I^0 \sigma_e / B) \delta(\mathbf{k} - \mathbf{k}' - 2\pi\boldsymbol{\tau}) + Q \sigma_i / 4\pi] \quad (7)$$

where B is the volume of a unit cell, and

$$2\pi\boldsymbol{\tau} = l_1 \mathbf{b}_1 + l_2 \mathbf{b}_2 + l_3 \mathbf{b}_3. \quad (7a)$$

Here l_1 , l_2 , and l_3 are integers; the \mathbf{b}_i are reciprocal lattice vectors.

$$I^0 = |\sum_n P(\mathbf{n}) \langle \mathbf{n} | I | \mathbf{n} \rangle|^2, \quad (7b)$$

$$Q = \sum_n [P(\mathbf{n}) - P(\mathbf{n})^2] |\langle \mathbf{n} | I | \mathbf{n} \rangle|^2, \quad (7c)$$

$$\sigma_e = (1/p) |\sum' \sigma_j^{\pm} \exp(i2\pi\boldsymbol{\tau} \cdot \mathbf{R}_j)|^2. \quad (7d)$$

In Eq. (7d) \mathbf{R}_j is the position of the j th nucleus in a unit cell; the sum runs over the unit cell; the sign of σ_j^{\pm} in general depends on j .

The δ -function, arising from the sum in (3a), is characteristic of crystal-diffraction problems and restricts scattering to the direction of the Laue spots. These directions are determined by the equation

$$\mathbf{k} - \mathbf{k}' = 2\pi\boldsymbol{\tau}. \quad (8)$$

Since $k = k'$, one has $2k \sin\theta/2 = 2\pi\tau$, and hence

$$\pi\tau \geq k. \quad (8a)$$

The second term in (7) gives rise to an isotropic, incoherent scattering, which disappears if the crystal is cooled to 0°K; it is introduced by the randomness of the initial state of an oscillator.

The polycrystalline elastic cross section is calculated by averaging the monocrystalline cross section over all orientations of the single crystal. This may be done by averaging over $\boldsymbol{\tau}$, since $\boldsymbol{\tau}$ is fixed relative to the axes of the single crystal. Finally the cross section is integrated over all scattering angles in the neighborhood of $\mathbf{k}' = \mathbf{k} + 2\pi\boldsymbol{\tau}$. The result is that the total cross section associated with a given value of τ is

$$\sigma^0 = (m_N/\mu)^2 [\pi \sigma_e I_0 / 2Bk^2 \tau + Q \sigma_i]. \quad (9)$$

The total-elastic polycrystalline cross section is obtained by summing (9) over all allowed

³ Reference 1, R. Weinstock.

directions. The result is

$$\sigma^0 = (\pi m_N^2 / 2\mu^2 B k^2) \sum_i^{\tau \leq k/\pi} I^0 \sigma_c / \tau. \quad (10)$$

The isotropic term is omitted from (10) because it vanishes if all oscillators are in their ground state, and in any case it is small.

4. THE SINGLE OSCILLATOR FUNCTIONS

The elastic and inelastic cross sections are given by Eqs. (10) and (6) respectively, but the one-oscillator functions appearing in them must now be calculated. These functions are based on the matrix element $(\mathbf{n}|I|\mathbf{n}')$ which is defined in Eq. (4) where

$$\varphi(\mathbf{u}, \mathbf{n}) = \varphi(u_x, n_x) \varphi(u_y, n_y) \varphi(u_z, n_z).$$

Hence $(\mathbf{n}|I|\mathbf{n}')$ can be broken into three factors, one of which is

$$(n_x|I|n_x') = \int_{-\infty}^{+\infty} \exp[i(k_x - k_x')u_x] \times \varphi(u_x, n_x) \varphi(u_x, n_x')^* du_x. \quad (11)$$

The φ are the oscillator wave functions

$$\varphi(u, n) = (\pi^{1/2} a 2^n n!)^{-1/2} \exp(-\frac{1}{2}\xi^2) H_n(\xi) \quad (11a)$$

where

$$\xi = u/a \quad \text{and} \quad a = (\hbar/m\omega)^{1/2}. \quad (11b)$$

Here m and ω are the mass and frequency of an average nucleus in the lattice. Let

$$\chi(\xi, n) = a^{1/2} \varphi(u, n). \quad (12)$$

Then use can be made of the result that the Fourier transform of the product $\chi(\xi, n)\chi(\xi, n')$ of two orthonormalized Hermite functions is an associated Laguerre function. That is,

$$\int_{-\infty}^{+\infty} e^{iq\xi} \chi(\xi, n) \chi(\xi, m)^* d\xi = (-)^{\frac{1}{2}(m-n)} \Phi_m^{(m-n)}(q^2/2) \quad \text{with } m > n \quad (13)$$

where

$$\Phi_{n+\lambda}^\lambda(x) = \frac{(n!)^{\frac{1}{2}}}{[(n+\lambda)!]^{\frac{1}{2}}} e^{-x/2} x^{\lambda/2} \frac{d^\lambda L_{n+\lambda}(x)}{dx^\lambda} \quad (13a)$$

and where $\lambda = m - n$. Here $L_n(x)$ is the n th Laguerre polynomial. The functions $\Phi_{n+\lambda}^\lambda$ are the

orthonormalized-associated Laguerre functions.⁴ Equation (13) can be proved as follows.

By use of the generating function

$$\exp(-t^2 + 2tx) = \sum H_n(x) t^n / n!$$

it is easily shown that

$$y = \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} \frac{t^n s^m}{n! m!} I_{nm} \quad (14)$$

where

$$I_{nm} = \int_{-\infty}^{\infty} \exp(-x^2) H_n(x) H_m(x) e^{iqx} dx$$

and

$$y = e^{2ts} \int_{-\infty}^{\infty} \exp[-(t+s-x)^2] e^{iqx} dx = \pi^{1/2} \exp(-q^2/4) e^{2ts+iq(t+s)}.$$

Hence

$$I_{nm} = \left(\frac{\partial^{n+m} y}{\partial t^n \partial s^m} \right)_{t=s=0} = \left[\frac{\partial^n}{\partial t^n} (2t+iq)^m y \right]_0.$$

By performing the indicated differentiations one now shows that y generates the Laguerre functions. In fact the required integral is

$$(\pi^{2n+2m} n! m!)^{-1/2} I_{nm} = [n!(n+\lambda)!]^{-1/2} \times \exp(-q^2/4) \sum_{\nu} \binom{n+\lambda}{\nu+\lambda} \frac{n!}{\nu!} \left(-\frac{q^2}{2}\right)^{\nu+\lambda/2}. \quad (15)$$

This last expression is readily identified with the Laguerre functions as stated in Eq. (13).

The required matrix elements are

$$(\mathbf{n}|I|\mathbf{n}') = (-)^{\frac{1}{2}(\lambda_x+\lambda_y+\lambda_z)} \Phi_{n_x}^{\lambda_x}(q_x^2) \times \Phi_{n_y}^{\lambda_y}(q_y^2) \Phi_{n_z}^{\lambda_z}(q_z^2) \quad (16)$$

where

$$\mathbf{q} = (a/\sqrt{2})(\mathbf{k} - \mathbf{k}'). \quad (16a)$$

Now the probability that the x -oscillator will be in the state n_x is

$$P(n_x) = z^{n_x} / \sum z^n = (1-z) z^{n_x} \quad (17)$$

where

$$z = \exp(-\hbar\omega/kT). \quad (17a)$$

But by (7b) and (16)

$$I^0 = (1-z)^2 \left| \left[\sum z^n \Phi_n^0(q_x^2) \right] \right|^2. \quad (18)$$

The square bracket in (18) is just the generating function of the Laguerre functions, i.e.,

$$\sum_0^{\infty} z^n \Phi_n^0(x) = (1/1-z) \exp[-x(1+z)/2(1-z)]$$

⁴ The integral (13) is calculated by Weinstock but the result is not identified as a Laguerre function.

so that

$$I^0 = \exp[-q^2(1+z)/(1-z)].$$

Since we are considering the case of elastic scattering we also have $\mathbf{q} = (a/\sqrt{2})2\pi\boldsymbol{\tau}$. Hence I^0 may be written

$$I^0 = \exp(-A\tau^2) \quad (19)$$

where

$$A = (\hbar^2/2mk\Theta) \coth(\Theta/2T). \quad (19a)$$

In (19a) k is Boltzmann's constant and Θ is the Einstein temperature of the lattice ($\hbar\omega = k\Theta$).

An exact calculation of the function I^\pm given in (6b) appears difficult, but may be avoided by use of the following approximations. To calculate the emission cross section assume that the initial state of the oscillator is always the ground state: $P(n) = \delta(n, 0)$. On the other hand, to calculate the absorption cross section assume that the final state of the oscillator is always the ground state. Under these assumptions the matrix elements for emission and absorption are equal: $(0|I|\mathbf{n}) = (\mathbf{n}|I|0)^*$.

The absorption cross section becomes important only for very slow neutrons. For these neutrons it varies with the energy, E , as $E^{-\frac{1}{2}}$ for the Einstein model and as E^{-1} for the Debye model. In this case the latter model is, of course, to be preferred; the Einstein picture fails here, as it does for specific heats, because it does not take account of low frequency vibrations. For this reason further discussion of absorption cross sections will not be given.

The calculation of J^- has been given elsewhere,² under the above assumption $P(n) = \delta(n, 0)$. The result, which is to be inserted in Eq. (6), is

$$J^- = \sum_1^{n \leq \epsilon} J_n^- \quad (20)$$

where

$$J_n^- = (m/4m_N\epsilon) [f_n(q_1^2) - f_n(q_2^2)], \quad (20a)$$

$$f_n(x) = e^{-x}(1+x+\dots+x^n/n!), \quad (20b)$$

$$q_1 = (m_N/m)^{\frac{1}{2}} [\epsilon^{\frac{1}{2}} - (\epsilon - n)^{\frac{1}{2}}], \quad (20c)$$

$$q_2 = (m_N/m)^{\frac{1}{2}} [\epsilon^{\frac{1}{2}} + (\epsilon - n)^{\frac{1}{2}}], \quad (20d)$$

$$\epsilon = E/\hbar\omega. \quad (20e)$$

Before discussing these results we consider the

case in which the harmonic-oscillator model of the crystal is not appropriate.

5. NEUTRON ENERGY LARGE COMPARED TO CHEMICAL BINDING ENERGY

If the energy absorbed by the scattering nucleus exceeds the energy by which it is bound to the crystal, then the collision ejects the nucleus from its original lattice site. To calculate the cross section for this event, assume for simplicity that the wave function of the final state of the nucleus is the unbound plane wave $\exp(i\mathbf{K}\cdot\mathbf{r})$ where $\hbar\mathbf{K}$ is the momentum of the free nucleus.

The relevant matrix element is now

$$(0|I|K) = (a^{3/2}/\pi^{3/4}) \int \exp(-\frac{1}{2}\xi^2 + ia\mathbf{S}\cdot\xi) d\xi \\ = (2a)^{3/2}\pi^{3/4} \exp(-\frac{1}{2}S^2a^2). \quad (21)$$

where

$$\mathbf{S} = \mathbf{k} - \mathbf{k}' - \mathbf{K}. \quad (21a)$$

\mathbf{S} is the momentum given to the lattice. The total probability for the ejection of the scattering nucleus into the continuous spectrum is determined by the following integral, which replaces the sum in (6b),

$$I^- = (1/32\pi^4) \int_{K_b}^{K_m} \int_0^{2\pi} \int_0^\pi (k'/k) |(0|I|\mathbf{K})|^2 K^2 \sin\omega d\omega d\alpha dK$$

where $\hbar\mathbf{K}_b$ is the momentum which a nucleus needs in order to escape from its position in the lattice and $\hbar\mathbf{K}_m$ is the maximum momentum which a nucleus can acquire in a collision with the neutron. Here (ω, α) is the recoil direction of the nucleus. The total cross section is by (6)

$$\sigma = (m_N/\mu)^2 \sigma_i (a^3/4\pi^{5/2}) \int_{K_b}^{K_m} \int_0^{2\pi} \int_0^\pi \int_0^\pi (k'/k) \\ \times \exp(-S^2a^2) \sin\omega d\omega d\alpha \sin\theta d\theta \varphi K^2 dK \quad (22)$$

where (θ, φ) is the recoil direction of the neutron. Integration over all recoil directions of the nucleus gives

$$\int_0^{2\pi} \int_0^\pi \exp(-S^2a^2) \sin\omega d\omega d\alpha \\ \cong (\pi/lKa^2) \exp[-(l-K)^2a^2] \quad (23)$$

where $l = \mathbf{k} - \mathbf{k}'$. (This last equation is approximate since it is based on the assumption $lKa^2 \gg 1$ or $\hbar^2 lK/2m \gg \hbar\omega/2$. This condition is well satisfied, however, since $l = |\mathbf{l}| = |\mathbf{S} + \mathbf{K}| \geq K$. Hence $\hbar^2 lK/2m \geq \hbar^2 K^2/2m \geq \hbar^2 K^2/2m$. But $\hbar^2 K^2/2m \gg \hbar\omega/2$. $\therefore \hbar^2 lK/2m \gg \hbar\omega/2$.) Put Eq. (23) in (22), and integrate over (θ, φ) . As the variable of integration it is convenient instead of θ to use

$$x = a(l - K).$$

The result is

$$\sigma = \sigma_i (m_N/2\mu k)^2 \int_{K_b}^{K_m} [\Phi(x_2) + \Phi(x_1)] K dK \quad (24)$$

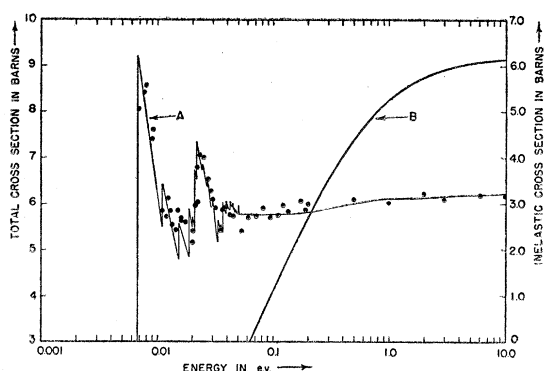


FIG. 1. Total cross section (Curve A) and inelastic cross section (Curve B) for the scattering of neutrons by microcrystalline Be. (Note the different scales for curves A and B.) Curve B actually intersects the energy axis with a vertical tangent and in addition has a discontinuous structure. These features are not shown in the figure because the discontinuities of slope contributed by both the elastic and inelastic cross sections have been smoothed out at higher energies.

where

$$x_2 = [k + k[1 - (m_N/m)(K/k)^2]^{1/2} - K]a, \quad (24a)$$

$$x_1 = [-k + k[1 - (m_N/m)(K/k)^2]^{1/2} + K]a, \quad (24b)$$

and Φ is the error function

$$\Phi(x) = (2/\pi^{1/2}) \int_0^x \exp(-x^2) dx. \quad (24c)$$

The maximum momentum which the recoiling nucleus can take from the incident neutron is

$$K_m = (m/m_N)^{1/2} k. \quad (24d)$$

This large value of K is allowed, but improbable, since the integrand of (24) is small unless momentum is conserved between neutron and nucleus alone. Equation (24) gives the cross section for collisions in which a nucleus is dislocated. The total cross section consists of (24) plus the contribution from (6) where the sum in (20) is, of course, only to be carried as high as the binding energy.

6. DISCUSSION OF RESULTS

By Eqs. (10) and (17) the total elastic cross section of an Einstein polycrystal is

$$\sigma^0 = (\pi m_N^2 / 2\mu^2 B k^2)$$

$$\times \sum_1^{\tau \leq k/\pi} \sigma_e(\tau) \tau^{-1} \exp(-A\tau^2). \quad (25)$$

The sum is extended over all triplets of integers $l = (l_1, l_2, l_3)$ not excluded by either the vanishing of σ_e or the maximum value of τ . Each term in the sum may be interpreted as expressing the scattering by a set of parallel planes (with Miller indices: l_1, l_2, l_3). Equation (25) agrees closely with the one deduced for a Debye crystal;⁵ the only difference is the expression for A (Eq. 17a), but even here the difference between the two formulas is insignificant. The factor $\exp(-A\tau^2)$ is in any case nearly unity; although even at $T=0$, it is not exactly unity because of the zero-point energy.

When the kinetic energy of the neutron is of the order of 1 volt, the sum in (25) is conveniently replaced by an integral, namely,

$$\sigma_i \int_0^{k/\pi} \tau^{-1} \exp(-A\tau^2) \rho(\tau) d\tau \quad (26)$$

where $\rho(\tau)d\tau$ is the number of points in 1-space inside of the ellipsoidal shell ($\tau, \tau+d\tau$). The equation of the ellipsoid, τ , is

$$\tau^2 = \sum (l_i \mathbf{b}_i)^2 = \sum l_i l_j \mathbf{b}_i \mathbf{b}_j.$$

Let the diagonal values of $|\beta_{ij}|$, where $\beta_{ij} = \mathbf{b}_i \cdot \mathbf{b}_j$, be β_1, β_2 , and β_3 . The volume of the ellipsoid associated with τ is $4\pi\tau^3/3(\beta_1\beta_2\beta_3)^{1/2}$. Hence $\rho(\tau) = 4\pi\tau^2/(\beta_1\beta_2\beta_3)^{1/2}$. But the invariant $\beta_1\beta_2\beta_3 = |\beta_{ij}| = B^{-2}$ where B is the volume of a unit cell. Hence $\rho = 4\pi B\tau^2$. Using this density in (26) one finds

$$\sigma^0 = (\sigma_i \pi^2 m_N^2 / \mu^2 A k^2) [1 - \exp(-A k^2 / \pi^2)]. \quad (27)$$

The elastic cross section given by (25) is a discontinuous function of neutron energy in the thermal region, but Eq. (27) obviously represents a continuous function in the region in which it is valid.

The inelastic cross section is given by Eqs. (6) and (20), for the case in which the scattering nucleus is not knocked out of its lattice site. For large ϵ and low n , Eq. (20) shows that

$$J_n = m/4m_n \epsilon. \quad (28)$$

Finally, if the scattering nucleus is dislocated, one uses (24) in conjunction with (6), (20), and (28). These equations may be combined to give

⁵ See the papers of Weinstock and Halpern, Hamermesh, and Johnson, reference 1.

the approximate formula, valid for large k ,

$$\sigma = \sigma_i \left[(m_N/2\mu k)^2 \int_{K_b}^{K_m} [\Phi(x_2) + \Phi(x_1)] K dK + (M/4\mu)(E_b/E) \right] \quad (29)$$

where $M = m + m_N$ and E_b is the binding energy.

Formula (29), of course, simplifies for large k . In fact, if $k \gg K \gg 1/a$, then $x_2, x_1 \gg 1$, so that $\Phi \cong 1$. Hence (29) becomes

$$\sigma \cong \sigma_i (m_N/2k\mu)^2 K_m^2. \quad (30)$$

It has been remarked in the previous section that momentum is usually conserved between neutron and nucleus alone, although there is a small probability that some momentum will be lost to the lattice. The improbability of transferring momentum to the lattice is clearly displayed in Eq. (21) which shows that the probability that the lattice acquires the momentum S is proportional to $\exp(-\frac{1}{2}S^2a^2)$, where a measures the tightness of the chemical binding. The same effect is brought out by the fact that the integrand of (29) is very small for values of K larger than

$$K_m = 2k\mu/m_N. \quad (31)$$

which is the limit correct for a two-body collision. The effective upper limit in (29) is therefore given by (31) and not (24d). Substitution of Eq. (31) into (30) then leads to the correct limiting condition

$$\sigma = \sigma_i.$$

In Fig. 1 the theoretical cross section for Be computed from Eqs. (6), (20), (24), (27), and (28) (and the constant $\Theta = 740^\circ\text{K}$) is compared with the experimental data.⁶ The data are compatible with a binding energy, E_b , of 3.3 volts, the cohesive energy of Be. Although the theoretical curve is not changed much if E_b is taken greater than this value, it is changed if E_b is taken much smaller; but the curve is not very sensitive to E_b . It should perhaps also be noted that the effect of binding is underestimated by our simplifying assumption that the final state of the struck nucleus is free; whereas it is overestimated by the other extreme assumption, $E_b = \infty$, according to which the final state is also bound.

The formulas obtained here for the inelastic cross section may be useful in an investigation of the slowing down of neutrons in crystalline materials. For example, the average energy loss in a collision is

$$\langle \epsilon \rangle_{Av} = \sum \epsilon (\sigma_\epsilon / \sigma)$$

where σ_ϵ is the cross section for losing the energy ϵ in a collision and where σ is the total cross section.

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⁶ E. Fermi, W. J. Sturm, and R. G. Sachs, Phys. Rev. **71**, 589 (1947). There the theoretical *elastic* cross section is compared with the data.