

crystalline axis. This fact seems to indicate that "the turning of the magnetization into the direction of the field" has to overcome mainly crystalline forces. Finally it has been pointed out by Becker and Doering³¹ that stresses sufficiently large to overcome the crystal orientation energy cannot be realized in iron since they would have to exceed the breaking strength of the material.

³¹ R. Becker and W. Doering, *Ferromagnetismus* (Julius Springer, Berlin, 1939), p. 104.

It should be emphasized as a guide for future experiments that it is not at all necessary to use completely polarized neutron beams for the investigation of the properties of ferromagnets. Polarizations as claimed to be present in the various experiments discussed would be amply sufficient to allow investigations of ferromagnetic structures.

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The Passage of Neutrons Through Crystals and Polycrystals

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We investigate in this paper phenomena, occurring in the passage of neutrons through matter, which originate from the crystalline or polycrystalline constitution. While the procedure is in many respects closely similar to that followed in the theory of x-rays, important and quantitatively decisive differences arise from the complicated coherence properties of the *atomic* scattering. The theoretical formulae developed in the first two paragraphs permit us to interpret in a quantitative manner a series of experiments which show deviations from the so far almost always assumed additivity of nuclear cross sections. We also obtain information concerning the relative phases of the scattering amplitudes of nuclear isotopes. We next show for illustrative purposes how the Larmor precession of the spin of the neutron passing through the magnetized medium, and the well-known differentiation between the

action of the vectors "B" and "H" can be explained as a simple dispersion phenomenon. The preceding formulae permit us to determine quantitatively the transmission and polarization of neutron beams passing through ferromagnetic bodies. The main uncertainties which enter into attempts to evaluate experiments, arise from our incomplete knowledge of the velocity distribution of the incident beam and of the form factor which enters into the formulae for magnetic scattering. We present a detailed discussion of these uncertainties. Even neglecting depolarization effects which are due to incomplete saturation and which would still further diminish the theoretical value for transmission effects, we find that the observed values are considerably higher than those theoretically predicted and are not in good agreement with each other.

INTRODUCTION*

CONTINUING earlier investigations¹ on the transmission of neutrons through macroscopic bodies, and in particular on macroscopic and microscopic magnetic effects, we present in this paper a discussion of the influence of crystal structure on scattering and polarization of neu-

trons. It has been the accustomed procedure to consider the nuclear cross section for the scattering of slow neutrons as a strictly additive property independent of the physical state or the chemical constitution of the sample investigated. On this basis the total cross section of a chemical compound could, for example, be determined from a knowledge of the cross sections of the constituent elements.

Such a procedure is valid only if we are dealing with a substance of strictly amorphous structure (a gas). In all other cases the crystalline structure of the material becomes significant; it will turn out to be of importance even for substances

* A preliminary report of this work appeared in the abstract: Halpern, Hamermesh and Johnson, *Phys. Rev.* **55**, 1125A (1939).

¹ I. O. Halpern and M. H. Johnson, *Phys. Rev.* **51**, 992 (1937); II. *ibid.* **52**, 52 (1937); III. *ibid.* **55**, 898 (1939); IV. Halpern and Holstein, *ibid.* **55**, 601 (1939); V. *ibid.* **59**, 960 (1941) (this issue). These are referred to throughout the paper by the corresponding Roman numerals.

composed of small microcrystals, and to change completely the scattering results for macroscopic crystals. The theory leading to these results is in its essentials the same as that for x-ray scattering, but shows great quantitative differences due to peculiarities which are characteristic of the interaction between neutron and atoms.

In discussing any crystal phenomenon it is essential to separate the coherent and incoherent scattering processes which have previously been found to play so great a part in the theory of x-ray scattering; but while the theory of x-ray scattering by a single chemical element had to take into account only those incoherent processes which are produced by inelastic collision of the incident particles with the lattice vibrations (strictly inelastic scattering), we have in the case of neutrons two more causes for incoherent processes. These are: first, the existence of spin dependent forces between the neutron and the atom, which may be of a nuclear or magnetic type; and secondly, the disorder in the lattice caused by the random distribution of the isotopes, which in general will produce scattered neutron waves, whose amplitude and phase will show no correlation for the various isotopes.

The second part of the paper is concerned with the quantitative evaluation of polarization experiments. We have previously² pointed out that the existing³ theories of polarization effects, which fail to take into account the crystalline structure as well as the various types of scattering, have no direct field of application, and that it is also necessary to calculate in detail the effect of incomplete ferromagnetic saturation on the intensity of the scattered and transmitted beam. We find that the previous estimates of polarization effects are of a higher order of magnitude than those obtained by the rigorous theory. These calculations of course have to be used together with the results of IV and V on magnetic depolarization.

Among previous investigations of the passage of neutrons through crystals, papers by Wick⁴ and Pomeranchuk⁵ may be mentioned. Pointing

out that the elastic scattering of neutrons does not offer much interest, since it is closely analogous to the problem in x-ray scattering, Wick shows that an essential difference arises in the inelastic scattering due to the interaction with the lattice vibrations. This difference arises from the nonrelativistic motion of the neutron (energy = momentum $\times V/2$, not momentum $\times V$ as in the x-ray case), which tends to reduce the inelastic scattering. Similarly, Pomeranchuk discusses mainly the slowing down of neutrons in crystals for neutrons of long wave-length. The physical aspects which are relevant in our paper have not been treated by these authors.

I. THE GENERAL SCATTERING FORMULAE FOR ATOMS

Before considering the effect of the crystalline structure of the scatterer on the results of transmission experiments we wish to review briefly the theory of the passage of neutrons through a material consisting of independent scatterers.

We shall be dealing throughout with slow neutrons, so that only the "s" wave need be considered; also inelastic nuclear scattering can be excluded since the energy of the neutron is too small to excite the nucleus to higher states. If one takes account of the different isotopes present in the scattering sample, the amplitude of the coherent scattering from a single nucleus is given by:⁶

$$C = \sum_p |b_p|^2 (2i_p + 1)^{-1} [i_p a_0^p + (i_p + 1)a_1^p], \quad (1.1)$$

where $|b_p|^2$ gives the relative abundance of the p th isotope, i_p is the nuclear spin of the p th isotope, and a_0^p and a_1^p are the amplitudes of the scattered wave for total angular momenta $i_p - \frac{1}{2}$ and $i_p + \frac{1}{2}$, respectively (neutron spin = $\frac{1}{2}$).

The intensity of the incoherent nuclear scattering is proportional⁶ to:

$$E^2 = \sum_p |b_p|^2 (2i_p + 1)^{-1} \times [i_p(i_p + 1)(a_1^p - a_0^p)^2]. \quad (1.2)$$

In addition to this purely nuclear scattering, there will be an interaction between the magnetic moment of the neutron and the magnetic field due to the current distributions of the electrons in the atom. Since in most cases one deals with

² Cf. V.

³ F. Bloch, Phys. Rev. **50**, 259 (1936); J. Schwinger, Phys. Rev. **51**, 544 (1937).

⁴ G. C. Wick, Physik. Zeits. **38**, 403, 689 (1937).

⁵ I. Pomeranchuk, Physik. Zeits. Sowjetunion **13**, 65 (1938).

⁶ See Sections III and VI of III.

materials in the crystalline state, the orbital currents are either absent (ground state S), or almost completely quenched by the crystalline field, so that the magnetic properties of the atom are due almost entirely to spin currents. For the amplitude of the magnetically scattered wave we have:⁶

$$\psi_m = \left(\frac{2\pi M_0}{hk}\right)^{\frac{1}{2}} \left(\frac{2e^2\gamma}{mc^2} F^{\frac{1}{2}}\right) \frac{e^{ikr}}{r} \times [(\mathbf{e} \cdot \mathbf{s})(\mathbf{e} \cdot \mathbf{S}) - (\mathbf{s} \cdot \mathbf{S})] \cdot X_s \Omega_M, \quad (1.3)$$

where M_0 = mass of the neutron; γ = its magnetic moment in nuclear magnetons;

$$\mathbf{e} = (\mathbf{k} - \mathbf{k}') / |\mathbf{k} - \mathbf{k}'|, \quad (1.4)$$

where \mathbf{k} and \mathbf{k}' are the initial and final propagation vectors of the neutron; \mathbf{s} is the spin of the neutron in units of $\hbar/2\pi$; X_s is the spin wave function of the incident neutron; $F^{\frac{1}{2}}$ is the form factor of the spin distribution of the ion, and Ω_M is the spin function describing the orientation of the spin S of the ground state of the ion. (The incident flux has been normalized to 1.)

In the case of ferromagnets at saturation, the spins of all the ions are rigidly aligned along a direction given by the unit vector \mathbf{k} .

In this case only elastic collisions in which the spin state of the ion is unchanged are possible, and the expression for the magnetically scattered wave becomes:⁶

$$\psi_m = (2\pi M_0/hk)^{\frac{1}{2}} 2Dr^{-1} e^{ikr} (\mathbf{q} \cdot \mathbf{s}) X_s, \quad (1.5)$$

where

$$D = \frac{e^2\gamma S}{mc^2} F^{\frac{1}{2}}, \quad (1.6)$$

$$\mathbf{q} = \mathbf{e}(\mathbf{e} \cdot \mathbf{k}) - \mathbf{k}. \quad (1.7)$$

Then the total coherently scattered wave (including both magnetic and nuclear scattering) becomes:⁶

$$\psi_{sc} = (2\pi M_0/hk)^{\frac{1}{2}} r^{-1} e^{ikr} (C + 2D\mathbf{q} \cdot \mathbf{s}) X_s. \quad (1.8)$$

In addition to the above scattering processes, there will be possible capture of the neutron which would lead to a decrease in intensity of the transmitted beam. The cross section σ_{cap} for this

straight absorption will for slow neutrons follow the $1/v$ law.

II. SCATTERING BY CRYSTALS AND AGGREGATES OF CRYSTALS

Before proceeding with calculations, we wish to fix the nomenclature to be used throughout.

The basic unit in the crystal is the unit cell which, by the repetition of a set of translations, fills out the whole space, forming a microcrystal.

The microcrystal is a composite of unit cells which are in perfect arrangement and scatter coherently.

A single crystal is composed of microcrystals all of which are oriented approximately the same, but whose relative positions are fixed only within a distance of the order of the lattice spacing. (Mosaic single crystal.) The single crystal will act macroscopically as a homogeneous body, but in the propagation of de Broglie waves of the order of the lattice spacing, the separate microcrystals will not scatter coherently. To calculate the scattering from the single crystal, we must first calculate the scattered amplitude for each of its microcrystals and then sum the intensities.

A polycrystalline material is composed of many small single crystals, or crystallites, oriented at random. The crystallites in general contain many microcrystals. To calculate the scattering from a polycrystalline sample, one must average the scattering of its sub-units over all orientations of the crystallites.

By the perfectness of a crystal we mean the linear dimension of the microcrystals composing it.

To calculate the total scattering from a polycrystalline sample, we must integrate the usual diffraction integral over all final directions of the neutron, and then average over all orientations of the constituent microcrystals.

We consider the nuclear scattering of neutrons of wave-length λ by a material having simple cubic structure with lattice distance a , and only one type of nucleus in the lattice. Using the well-known relation

$$2 \cos\theta_0 = |l| \lambda / a \quad (2.3)$$

$$l = (l_x^2 + l_y^2 + l_z^2)^{\frac{1}{2}}; \quad l_i \text{ Miller indices,}$$

one obtains⁷ for the scattering due to "reflection"

⁷ A. H. Compton and S. K. Allison, *X-Rays in Theory and Experiment* (Van Nostrand, 1935).

from the plane l_i

$$I_i = \frac{\sigma}{4\pi} \frac{N_1 N_2 N_3}{4} \left(\frac{\lambda}{a}\right)^3 \frac{1}{\cos\theta_0} \\ = \frac{N_1 N_2 N_3}{8\pi} \sigma \left(\frac{\lambda}{a}\right)^2 \frac{1}{|l|}. \quad (2.6)$$

In (2.6) σ is the cross section for the coherent scattering $=4\pi C^2$ (Section 1.1); N_1, N_2, N_3 are the numbers of planes in the microcrystal along each of the crystal axes. Finally this is to be summed over all triples for which $|l| < 2a/\lambda$.

$$I = \frac{N\sigma}{8\pi} \left(\frac{\lambda}{a}\right)^2 \sum_{|l| < 2a/\lambda} \frac{1}{|l|}, \quad (2.8)$$

where N is the total number of unit cells.

Before considering this fundamental formula in detail, we wish to examine the case where the initial beam is sharply defined and is incident exactly at the Bragg angle, and calculate the total scattering for this fixed orientation of the crystal. In this case we expect the scattering to be large. This is of interest in examining the influence of secondary extinction, a term which refers to the fact that the incident beam, in going through the specimen, is being depleted due to scattering from individual microcrystals, so that low lying microcrystals are shielded from the full intensity of the beam by microcrystals lying above them. This effect will be noticeable if the scattering of the given wave-length in the specimen is large, so to estimate its importance we choose this most favorable case of incidence at the Bragg angle. Also, for simplicity, we consider the microcrystals to be perfectly aligned, but nevertheless scatter incoherently. Slight variations in orientation would produce a broadening of the range of reflection, but have little effect on the final result.

This calculation seems impossible to perform analytically, but for our purposes only a rough estimate is needed. Each term in (2.8) represents the scattering for a given reflection averaged over all possible orientations. Since the range of initial directions in which scattering occurs appreciably is $\sim \lambda/a_i N_i$, we can take as a rough estimate of the scattering at the Bragg angle

$$N_i^4 \frac{\sigma \lambda}{8\pi a} \frac{1}{|l|} \quad (2.9)$$

so, for a beam incident exactly at the Bragg angle, the total scattered intensity should be proportional to N_i^4 . If the microcrystals have sides l , then the scattering will be

$$\sim \frac{l^4 \sigma \lambda}{8\pi a^5} \frac{1}{|l|}. \quad (2.10)$$

If the single crystal (crystallite) is L cm on a side, the ratio of scattered to initial beam will be:

$$\frac{I}{I_0} = \frac{1}{L^2} \left(\frac{L}{l}\right)^3 \frac{l^4}{8\pi a^5} \frac{\sigma \lambda}{|l|} \\ = \frac{L l \sigma \lambda}{8\pi a^5 |l|} \sim N^2 \sigma \lambda^2 l L. \quad (2.11)$$

For Fe, a rough estimate of the effect can be made: l is 10^{-5} cm, while the size of the crystallites is $L \sim 2 \times 10^{-3}$ cm.

$\sigma = 7.3 \times 10^{-24}$ cm² (the reason for this choice will be seen in Section III).

$$a = 2.9 \times 10^{-8} \text{ cm}, \quad \lambda = 1.5 \times 10^{-8} \text{ cm}.$$

Using these values we obtain:

$$I/I_0 = Ll(1.2/4) \times 10^6 \sim 6 \times 10^{-3}. \quad (2.12)$$

So even in this favorable case of reflection exactly at the Bragg angle, the secondary extinction will be very small for polycrystalline iron. Only for large single crystals ($L \sim 1$ cm) will it be important. In what follows we shall deal chiefly with polycrystalline samples for which we may neglect the extinction.

Equation (2.8) has been obtained for the scattering of neutrons of a single wave-length by crystals of simple cubic structure. In (2.8) we have not included the effect of the temperature motion of the nuclei in the crystal. The theory of this temperature motion has been given by Debye and Waller.⁸ The effect of the thermal vibration is to decrease the coherent scattering of a crystal of cubic symmetry by the factor

⁸ P. Debye, Ann. d. Physik **43**, 49 (1914); I. Waller, Zeits. f. Physik **51**, 213 (1928); Dissertation Uppsala (1925).

$\exp(-2M_w)$ where:

$$M_w = \frac{6h^2}{m_a k \Theta} \left[\frac{\varphi(x)}{x} + \frac{1}{4} \right] \frac{\sin^2 \frac{1}{2} \theta}{\lambda^2}, \quad (2.13)$$

where θ is the angle between final and initial direction of the beam, m_a = mass of the atom forming the lattice, k is the Boltzmann constant, $\varphi(x)/x$ is the Debye function, and $x = \Theta/T$, where Θ is the Debye temperature and T the absolute temperature of the crystal. For the reflection corresponding to index $|l|$, we have $|l|\lambda/2a = \sin \frac{1}{2} \theta$, so the factor giving the decrease in coherent scattering from the crystal becomes

$$\exp(-A|l|^2), \quad (2.14.1)$$

where

$$A = \frac{3h^2}{m_a k \Theta} \frac{1}{a^2} \left[\frac{\varphi(x)}{x} + \frac{1}{4} \right]. \quad (2.14.2)$$

It should be noted that the temperature factor does not depend on the wave-length; for a given Debye ring (definite $|l|$) it is the same for all wave-lengths. The $\frac{1}{4}$ represents the effect of the zero-point vibration.

For Fe, $\Theta = 453^\circ$,

and taking $T = 302^\circ$, $x = 1.5$,

$$\varphi(x) = 0.70, \quad \frac{\varphi(x)}{x} \sim 0.46; \quad \left[\frac{\varphi(x)}{x} + \frac{1}{4} \right] \sim 0.71.$$

Also for Fe, taking $a = 2.86\text{A}$; $m_a = 56 \times 1.661 \times 10^{-24}$ g we get $A = 0.0194$ so the temperature factor for iron becomes

$$\exp(-0.0194|l|^2). \quad (2.14.3)$$

As the index $|l|$ of the Debye ring increases the coherent scattering is cut down more and more; for $|l| = 4$, the factor is already 0.73.

In the case of Fe, a second correction must be made. Fe, at room temperature, forms a body-centered cubic lattice, with two atoms to each unit cell. This introduces a crystal structure factor which has the following effect:

All reflections for which $\sum_i l_i$ is odd disappear; all for which $\sum_i l_i$ is even are quadrupled in intensity. (We shall refer to these as odd and even $|l|$, respectively.)

In our scattering formula for simple cubic

lattice the factor N which gave the number of unit cells represented also the total number of atoms in the crystal, whereas for the body-centered case, the number of unit cells = $\frac{1}{2}$ the number of atoms. Our formulae will be correct for body-centered lattices if we use N to designate the number of atoms in the lattice and take

$$2 \sum_{\text{even } |l| < 2a/\lambda}$$

Then the final scattering formula becomes for simple cubic lattice:

$$\frac{N\sigma \left(\frac{\lambda}{a}\right)^2}{8\pi} \sum_{|l| < 2a/\lambda} \frac{\exp(-A|l|^2)}{|l|} \quad (2.15)$$

and for body-centered lattice (e.g. Fe)

$$2 \cdot \frac{N\sigma \left(\frac{\lambda}{a}\right)^2}{8\pi} \sum_{\text{even } |l| < 2a/\lambda} \frac{\exp(-A|l|^2)}{|l|}. \quad (2.16)$$

We see that the contributions to the total coherent scattering of the polycrystal from different rings decreases with increasing $|l|$ due to each of the factors in the summand. A given value of $|l|$ can be realized in many different ways; e.g., $|l| = \sqrt{2}$ can be gotten for (0, 1, 1); we must count all permutations and changes of sign in finding the multiplicity $j(|l|)$ of a term in the sum; for

$$|l| = \sqrt{2}, \quad j(|l|) = 12.$$

Since there have not yet been made significant experiments with monochromatic beams of slow neutrons it is necessary to generalize the formulae given for the case of rather wide velocity spectra. We shall in this section present some calculations *made for illustrative purposes only* by using a Maxwellian distribution. In Sections VI and VII calculations will be presented using empirically determined distribution functions.

In the case of a Maxwell distribution, the calculations can be carried out analytically; we so find for the scattered intensity produced by a body-centered lattice:

$$2 \cdot \frac{N\sigma \left(\frac{\lambda_A}{a}\right)^2}{4\pi} \times \sum_{\text{even } |l|} \frac{\Phi(\lambda_A |l|/2a) \exp(-A|l|^2)}{|l|}, \quad (2.17)$$

where

$$\Phi(x) = \frac{2}{\sqrt{\pi}} \int_x^\infty \exp(-y^2) dy \quad (2.17.1)$$

and

$$\lambda_A = h/(2M_0kT)^{1/2}, \quad (2.17.2)$$

where T is the temperature of the neutron source.

So the effective coherent cross section $\bar{\sigma}$ of the crystal, as determined by using a beam of thermal neutrons, will be related to the coherent cross section for independent nuclei σ by:

$$\frac{\bar{\sigma}}{\sigma} = 2 \cdot \frac{1}{4\pi} \left(\frac{\lambda_A}{a}\right)^2 \times \sum_{\text{even } |l|} \frac{\Phi(\lambda_A |l|/2a) \exp(-A |l|^2)}{|l|}. \quad (2.18)$$

These scattering formulae will be applied to the evaluation of experimental results in Section III.

Let us consider limiting cases for the various scattering formulae. (We consider only simple cubic lattices; similar arguments hold for crystals with basis.)

In (2.8), we can approximate the lattice sum by an integral; this gives

$$\frac{\bar{\sigma}}{\sigma} = \frac{1}{8\pi} \left(\frac{\lambda}{a}\right)^2 \int_0^{2a/\lambda} 4\pi l dl = 1.$$

The validity of this approximation by integral increases with increasing number of lattice points, i.e., decreasing λ . So for small λ , we find the effect of the crystal structure disappearing, as is to be expected from general reasoning.

In Eq. (2.15), where the effect of the temperature vibration is included, this limiting case gives a quite different result. Here replacing the sum by an integral gives

$$\frac{\bar{\sigma}}{\sigma} = \left(\frac{\lambda}{2a}\right)^2 \frac{1}{A} (1 - \exp(-(2a/\lambda)^2 A)),$$

so that as $\lambda \rightarrow 0$, $\bar{\sigma}/\sigma \rightarrow 0$. Again this result is easily interpreted. The inclusion of the temperature effect means the introduction of a form factor for the nuclear position in the crystal; any form factor $\rightarrow 0$, for $\lambda \rightarrow 0$.

In the expression for simple cubic crystals corresponding to (2.18), let us consider the case

where $\lambda_A \rightarrow 0$. The approximation by integral gives

$$\begin{aligned} \frac{\bar{\sigma}}{\sigma} &= \frac{1}{4\pi} \left(\frac{\lambda_A}{a}\right)^2 \int_0^\infty 4\pi l^2 \frac{\Phi(\lambda_A l/2a)}{l} dl \\ &= 4 \int_0^\infty v \Phi(v) dv \end{aligned}$$

and integration by parts gives $\bar{\sigma}/\sigma = 1$.

Let us consider (2.8) as λ increases. With increasing λ the number of terms in the sum decreases, but the intensity of each ring increases as λ^2 . As λ increases, there will be definite points at which Debye rings disappear. (The $|l|$ 'th will disappear at $\lambda = 2a/|l|$), and a discontinuous drop in intensity occurs; then because of the λ^2 factor, the intensity increases until the next Debye ring is cut out. If $\lambda > a$, only the first Debye ring is left and

$$\frac{\bar{\sigma}}{\sigma} \rightarrow \frac{1}{8\pi} \cdot e^{-A} \times j(1) = \frac{3e^{-A}}{\pi}, \quad \text{as } \lambda \rightarrow 2a.$$

For $\lambda > 2a$, the coherent scattering disappears completely.

Apart from the coherent scattering we have to discuss two types of incoherent scattering which form a background between the Debye rings. There is first the inelastic scattering originating from processes involving energy transfer between the neutron and the lattice. This inelastic scattering is, in the case of x-rays, given by formulae analogous to:

$$\sigma(1 - e^{-2Mw}) d\Omega. \quad (2.19)$$

In the case of neutrons conditions are more difficult, as mentioned already in the introduction. The inelastic cross section which would already be small for x-rays in case the Debye temperature is considerably larger than the temperature of observation becomes of even less significance for the scattering of slow neutrons.

The incoherent background due to the presence of isotopes constitutes a phenomenon which, with x-rays, is not of great importance numerically. It is due to the fact that the scattering amplitudes of various isotopes constituting the crystal have, in general, different magnitude as well as different sign. The spherically symmetrical background is produced with a scattering cross section

given by⁹

$$\sum_p |b_p|^2 \left[\frac{i_p a_0^p + (i_p + 1) a_1^p}{2i_p + 1} \right]^2 - \left(\sum_p |b_p|^2 \left[\frac{i_p a_0^p + (i_p + 1) a_1^p}{2i_p + 1} \right]^2 \right) + \sum_p |b_p|^2 \frac{i_p(i_p + 1)(a_1^p - a_0^p)^2}{(2i_p + 1)^2}. \quad (2.20)$$

We shall see later on that it probably accounts for the larger part of incoherent scattering occurring in so well-analyzed a substance as Fe.

III. DISCUSSION OF SCATTERING EXPERIMENTS

The deliberations of Section II contain the theoretical basis for the explanation and evaluation of scattering experiments. In particular, they give account of certain characteristic phenomena which were observed when neutrons were scattered from the same substances present either in different crystal forms or in different chemical combinations.¹⁰

We shall first discuss the observations made with Fe, since they will turn out to be of great importance not only for the evaluation of scattering experiments, but also for the quantitative determination of the polarization effects in ferromagnets as given in Section VI.

Experiments were performed first on a polycrystalline sample ($\sigma_{\text{polycr.}} = 12.0 \pm 0.2 \times 10^{-24} \text{ cm}^2$) and then on a single crystal of Fe ($\sigma_{\text{single cr.}} = 7 \times 10^{-24} \text{ cm}^2$), using a thermal distribution of neutrons at room temperature. The case of the single crystal may be described as follows: The resolving power of the microcrystals, which are all oriented in approximately the same direction, will limit the scattering to small regions in the neighborhood of those wave-lengths for which Bragg reflection occurs. These neutrons, for which the coherent scattering is large, represent only a small fraction of the total incident neutron intensity; hence for the entire incident neutron

beam, the effective coherent scattering will be negligibly small.

Thus the difference between the results in the two cases represents just the coherent scattering of the incident distribution by the polycrystalline sample. This gives for the effective coherent cross section $\bar{\sigma} = 5 \times 10^{-24} \text{ cm}^2$.

The ratio $\bar{\sigma}/\sigma$ with the temperature factor included has been calculated numerically for iron, with thermal neutrons. Using this calculated ratio $\bar{\sigma}/\sigma = 0.81$, and the experimental value of Whitaker and Beyer $\bar{\sigma} = 5 \times 10^{-24} \text{ cm}^2$ we find $\sigma = 6.25 \times 10^{-24} \text{ cm}^2$, so the nuclear amplitude

$$C = (\sigma/4\pi)^{1/2} = 7.05 \times 10^{-13} \text{ cm}.$$

We can similarly understand on the basis of our formulae the small deviations found by Whitaker and Beyer when the cross section of certain molecules was compared with the sum of the cross sections of the components. No general predictions can be made as to the sign of this effect, but since the crystal cross section for reasonable velocity distributions of the neutrons may differ by approximately 20 percent from the value for the amorphous state we can readily see that change of lattice, of basis, and of temperature factor can lead to cross-section changes of the order of magnitude of 10 percent. One must also keep in mind that some of the components (e.g., Cu) may possess rather large microcrystals and therefore show a partial extinction effect which will disappear when Cu enters into the chemical compound.

Similarly, in the case of alloys (e.g., Permalloy investigations by Whitaker and Beyer,¹⁰ and Nix, Beyer, and Dunning¹¹) the presence of an ordered crystalline structure should produce marked changes in the coherent scattering, and give rise to deviations from additivity; changes in the percentage composition, or treatment which break up the ordered crystalline structure should then lead back to the value given by additivity.

On the basis of our previous discussion, the current belief that the scattering cross section for slow neutrons is independent of the neutron energy can no longer be accepted. The ratio $\bar{\sigma}/\sigma$ has been calculated by use of expression (2.16) for Fe for monochromatic beams of vary-

⁹ The first two terms alone represent the incoherent scattering due to isotope disorder; the last term is due to spin dependence of nuclear forces. (See Section III of III; and reference 5.)

¹⁰ M. D. Whitaker and H. G. Beyer, Phys. Rev. **55**, 1101 (1939).

¹¹ Nix, Beyer and Dunning, Phys. Rev. **57**, 566A (1940).

ing wave-length. The results are plotted in Fig. 1. As already mentioned in Section II, increasing wave-length will mean a decrease in the number of Debye-Scherrer rings, but the intensity of each remaining ring goes up as λ^2 . Iron with lattice distance 2.86\AA is body-centered, so that the lowest order appearing will be $(1, 1, 0)$ with $|l| = \sqrt{2}$ and $j(|l|) = 12$; the coherent scattering from iron disappears for $\lambda > 2a/\sqrt{2} = 4.04\text{\AA}$. The limiting value for the coherent scattering at room temperature as $\lambda \rightarrow 4.04\text{\AA}$ is, from (2.18)

$$\bar{\sigma}/\sigma = (2/8\pi)2 \cdot e^{-2A} \cdot 12 = 1.29.$$

IV. DISCUSSION OF THE SIZE OF MICROCRYSTALS AND ESTIMATE OF THE SCATTERING AMPLITUDE OF Fe ISOTOPES

It is of interest to see that the preceding formulae, together with the observations of the difference in cross sections for the crystal and polycrystalline state of iron, enable us to draw some conclusions about the size of the microcrystals and the scattering amplitudes of the Fe isotopes.

For a rough discussion, it is sufficient to describe the weakening of a beam passing through an aggregate of crystallites as follows: The beam will be reduced in intensity by the factor $\exp(-\mu')$ where $\mu' = Ll\sigma\lambda/8\pi a^5$ (see (2.11)) when it strikes a crystallite at the Bragg angle. The probability of such an event is given by a/l , which represents the resolving power of the perfect microcrystal. This probability must be multiplied by a factor which gives the number of possible strong reflections for one and the same wave-length. Although only a *rough estimate* of this factor can be made, it is sufficiently accurate for our purposes to put it equal to 15. The total weakening of a beam is now determined by the various mutually exclusive alternatives that the beam strike 0, 1, 2, etc., properly oriented crystallites when passing through a thickness d of the substance. The probability of n favorable encounters is given by: $P_n = e^{-\alpha}\alpha^n/n!$ where $\alpha = 15ad/lL$ (Poisson formula). Denoting the size of one crystallite by L , we obtain for the intensity transmitted:

$$I = I_0 \sum_{n=0}^{\infty} P_n \exp(-n\mu') \\ = I_0 \exp[-\alpha(1 - \exp(-\mu'))]. \quad (4.1)$$

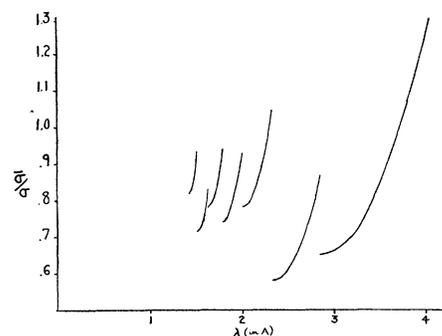


FIG. 1. Variation of crystalline cross section as a function of neutron wave-length.

This must be compared with the experimentally found absorption law $I = I_0 \exp(-N\bar{\sigma}d)$ where $\bar{\sigma}$ refers only to the coherent cross section of the polycrystal. Now two alternatives are possible: Case (1): $\exp(-\mu') \rightarrow 0$ (large extinction). In this case $I = I_0 e^{-\alpha}$ so $15ad/lL = N\bar{\sigma}d$. Using the empirically determined value $\bar{\sigma} = 5$ (see Section III), we obtain as an upper limit, $l \sim 5 \times 10^{-4}$ cm.

This upper limit for the size of the perfect microcrystal is, of course, highly exaggerated. It takes its maximum in the case of large extinction since the weakening of the beam by passing through one crystal grain is then almost complete. *It is also of interest to point out that in the case of marked extinction no polarization effect could be observed, since it is due to the slight increase or decrease of the atomic cross section produced by the interference of nuclear and magnetic scattering. If the nuclear scattering is already so large as to produce extinction, a slight change in the total atomic cross section cannot be of importance. A single crystal as distinguished from a polycrystalline body has complete extinction, and therefore cannot give an observable polarization effect.*

Case (2): This corresponds to the absence of extinction or, quantitatively speaking, $\exp(-\mu') \sim 1$. Since the numerator in

$$\exp[-15(ad/lL)(1 - \exp(-\mu'))]$$

is now very much smaller, the number of layers of the perfect microcrystal must be correspondingly reduced in order to keep the value for the scattering constant, and equal to the observed $\exp[-N\bar{\sigma}d]$. In the limiting case $\exp(-\mu') = 1 - \mu'$, the expression for the absorption reduces

to $\exp(-\alpha\mu') = \exp(-15\sigma\lambda d/8\pi a^4)$, and so becomes, as was to be expected, independent of the size of the microcrystal. This case corresponds to the condition found in nature, and leads to a value of $\sigma = 17 \times 10^{-24}$ cm². Since this case is precisely the one which we considered in Section II, the fact that the values of σ obtained by both arguments agree so closely, considering the roughness of the estimate, would indicate that our choice of some of the constants used is correct.

Recently, Miller and Du Mond¹² have given estimates of the length of perfect lattice in Ag and Al of approximately 500 lattice distances. They also find that after distortion and working the length is reduced to 150 to 200 lattice distances. Similar behavior in Fe would lead to negligible extinction.

We can also attempt to evaluate *approximately* the coherent cross section of the two iron isotopes which are present in the ratio of 92 : 8.¹³ Since the total *cross section of iron* is found to be 12 nuclear units (i.e., $12 \times 10^{-24} \times \text{cm}^2$) and the capture cross section to be approximately 3.5 n.u., we have to account for 8.5 units as being due to coherent and incoherent scattering. Of this, 5 n.u. are found to be coherent scattering, while the incoherent contribution of 3.5 n.u. is due to three causes: inelastic scattering by the lattice, incoherent nuclear scattering, and background due to isotope disorder. The inelastic scattering is small, while the incoherent nuclear scattering also probably does not contribute much to the total background. The isotope Fe⁵⁶ has probably no spin, being a $4n$ nucleus, while the isotope Fe⁵⁴ would have to have an anomalously large cross section to contribute a large portion of the observed background since it forms only 8 percent of the element. Lumping together these first two causes, and ascribing to them for purposes of a rough estimate a cross section of one nuclear unit, we obtain a value of 2.5 nuclear units for the disorder contribution as given by $\sum C_p f_p^2 - (\sum C_p f_p)^2$ where C_p is the concentration and $f_p = (4\pi)^{1/2} \times$ the coherent amplitude of the p th isotope, which for the case of two isotopes

reduces to

$$C_1 C_2 (f_1 - f_2)^2. \quad (4.2)$$

According to Section III, a crystalline cross section of five nuclear units corresponds to an amorphous cross section of approximately seven nuclear units. We can, with these data, attempt to determine the scattering amplitude and phase for the two isotopes. The equations are:

$$(0.92f_1 + 0.08f_2)^2 = 7 \quad (0.92)(0.08)(f_1 - f_2)^2 = 2.5.$$

There is no restriction of generality in assuming that the amplitude of the abundant isotope shall have the positive sign. We then obtain the following two sets of solutions for the amplitudes:

$$\text{either} \quad (\text{a}) \quad f_1 = 3.11; \quad f_2 = -2.72$$

$$\text{or} \quad (\text{b}) \quad f_1 = 2.18; \quad f_2 = 8.01.$$

(b) may be excluded as being highly improbable; it would lead to an unusually high cross section of 65 n.u. for the less abundant isotope Fe⁵⁴. We finally obtain the following estimate for the coherent cross sections of the two nuclei:

$$\text{Fe}^{56}: \quad \sigma \sim 9.7 \text{ n.u.}$$

$$\text{Fe}^{54}: \quad \sigma \sim 7.4 \text{ n.u.}$$

In addition to this, it should be noted *that the amplitudes have opposite signs.*

V. AN INTERPRETATION OF THE LARMOR PRE- CESSION OF THE SPIN DURING PASSAGE THROUGH MAGNETIZED MEDIA

We wish now to apply our results to the propagation of neutrons in a ferromagnetic medium (Fe), magnetized to saturation, with the spins of all ions rigidly aligned along the direction of a unit vector \mathbf{k} .

The total scattered wave from an ion will be given by (1.8):

$$\psi_{sc} = (2\pi M_0/hk)^{1/2} r^{-1} e^{ikr} (C + 2D\mathbf{q} \cdot \mathbf{s}) X_s.$$

The presence of the magnetic term introduces the possibility of changes in polarization due to the difference in scattering of the two spin states of the neutron. To put the possibility of such rotation of the plane of polarization clearly in evidence, let us consider a neutron beam of wavelength λ traversing a lattice whose spacing is less

¹² P. H. Miller and J. W. M. Du Mond, Phys. Rev. **57**, 198 (1940).

¹³ Actually, Fe has four stable isotopes. The concentration of Fe⁵⁸ is negligible; Fe⁵⁴ and Fe⁵⁷ have been lumped together and are referred to as "Fe⁵⁴."

than $\frac{1}{2}\lambda$. Then no Bragg maxima can occur and the coherent scattering is confined to the forward direction. We shall resolve the spin along the direction of the magnetization, which is the most convenient representation.

Suppose \mathbf{k} along the x axis; then \mathbf{q} has components $(e_x^2 - 1, e_x e_y, e_x e_z)$. Then, in summing over the lattice, the cross terms drop out because of the symmetry of the crystal, and only the x component ($||$ to \mathbf{k}) remains. We conclude that no depolarization can be produced by this process.

Nevertheless, the two polarization states are scattered differently. We shall treat the propagation of each of the polarization states as in classical dispersion theory by adding to the incident wave at any point the scattered waves from the centers in the medium, and determine an index of refraction. For simplicity, let the plane OXY contain one scattering center per unit area (see Fig. 2). Let \mathbf{k} be along the z axis. We must calculate the total wave at the field point P , where $OP = a$.

$$\begin{aligned} \mathbf{k} &= (0, 0, 1) \quad dx dy = a^2 \sec^2 \theta \tan \theta d\theta d\varphi \\ \mathbf{e} &= (1/2 \sin \frac{1}{2} \theta) (-\sin \theta \sin \varphi, -\sin \theta \cos \varphi, 1 - \cos \theta) \\ \mathbf{q} &= \frac{1}{2} (-\sin \theta \sin \varphi, -\sin \theta \cos \varphi, -\{1 + \cos \theta\}). \end{aligned}$$

The magnetically scattered wave from plane OXY is:

$$2D \int \int \frac{e^{i\mathbf{k}\cdot\mathbf{r}}}{r} (\mathbf{q} \cdot \mathbf{s}) dx dy X_s =$$

where $r = QP$

$$= 2Da^2 \int \int \sec^2 \theta \tan \theta d\theta d\varphi \frac{e^{ika \sec \theta}}{a \sec \theta} (\mathbf{q} \cdot \mathbf{s}) X_s.$$

As we have seen previously, only the z component remains, giving:

$$\begin{aligned} 2D\pi a \int_0^{\pi/2} \sec \theta \tan \theta d\theta e^{ika \sec \theta} (1 + \cos \theta) (\pm \frac{1}{2}) \\ = \pm \frac{D\pi}{ik} \int_0^{\pi/2} d(e^{ika \sec \theta}) (1 + \cos \theta). \end{aligned}$$

The integral will be oscillatory at the upper limit, as in all Fresnel diffraction problems, but just as in the optical case, such convergence difficulties can be eliminated by the introduction

of a weight factor. Partial integration gives:

$$\pm D \left[\frac{2\pi}{ik} e^{ika} + \frac{\pi}{ik} \int_0^{\pi/2} e^{ika \sec \theta} \sin \theta d\theta \right].$$

The second term

$$= -\frac{\pi a}{i} \int_{ka}^{\infty} \frac{e^{iy}}{y^2} dy;$$

we proceed neglecting this term. If we had included the nuclear part, this scattered wave from plane OXY would be:

$$\frac{2\pi}{ik} \left(C \pm \frac{e^2 \gamma S}{mc^2} \right) \psi_{inc}$$

for the two polarization states. But the total wave at point P will be the sum of the incident wave at P and the scattered waves from all planes below P . If the phase of the incident wave at P is taken at zero, its phase at OXY is e^{-ika} . So for a thickness d , the amplitude of the total wave is

$$\begin{aligned} I \left(1 + \frac{2\pi d}{ik} \left\{ C \pm \frac{e^2 \gamma S}{mc^2} \right\} \right) \\ = I \exp \left[-2\pi i \frac{d}{k} \left(C \pm \frac{e^2 \gamma S}{mc^2} \right) \right], \end{aligned}$$

where I is the incident wave, and we have assumed one scattering center per unit volume. This gives for the index of refraction:

$$n_{\pm} = \frac{2\pi}{k} \left(C \pm \frac{e^2 \gamma S}{mc^2} \right)$$

and for the rate of rotation of the direction of polarization: $(n_+ - n_-)$ (velocity of the beam)

$$= \frac{2\pi}{k} \frac{2e^2 \gamma S}{mc^2} \frac{\hbar k}{M_0} = \frac{4\pi e^2 \gamma S \hbar}{M_0 mc^2}. \quad (5.1)$$

From the macroscopic viewpoint, this rate of rotation should be given by the velocity of the Larmor precession of the neutron in the macroscopic field of the crystal. The magnetic moment/unit volume is $\mathbf{M} = e\hbar S/mc$ so that (5.1) becomes:

$$4\pi e \gamma \mathbf{M} / M_0 c. \quad (5.2)$$

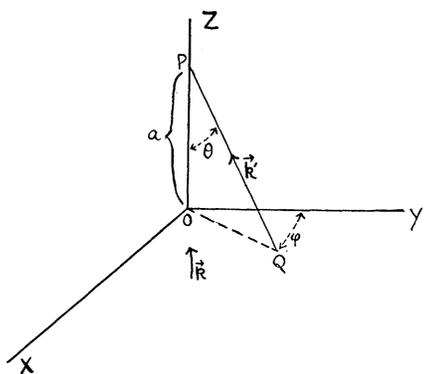


FIG. 2.

The total rotation of the plane of polarization is, of course, obtained by adding to (5.2) the precession due to the over-all magnetic field H . After adding this term which cannot be specified without knowledge about accidental outside fields, as well as the shape of the body, we can summarize the results by saying that it is the vector:

$$\mathbf{B} = \mathbf{H} + 4\pi\mathbf{M}, \quad (5.3)$$

which determines the total Larmor frequency of precession. Our derivation allows some insight into the manner and the mechanism by which the inhomogeneous magnetic field of the individual atoms averages out and leads to the well-known result for the rotation of the plane of polarization.

It can be shown easily that an analogous result holds when the direction of magnetization is no longer assumed to be parallel to the direction of incidence but allowed to make an arbitrary angle with it.

VI. POLARIZATION EXPERIMENTS WITH FERROMAGNETS; GENERAL PRINCIPLES AND CHOICE OF FORM FACTOR

Polarization effects accompanying the passage of neutrons through ferromagnets are due solely to the *interference* between nuclear and magnetic scattering. Since it was proven that the magnetic scattering by free electronic spins is always incoherent¹⁴ we have to limit the discussion to the case in which the electronic spin remains unchanged during the collision process. This is the case only for ferromagnets, and neutrons of

sufficiently small velocity. Similarly, only the coherent part of the purely nuclear scattering is relevant. Neither the incoherent nuclear scattering (i.e., transition with change of spin of nucleus) nor the background due to isotope disorder contribute anything to the magnetic polarization phenomenon; this is true for the latter since the magnetic scattering amplitude is the same for all isotopes, and therefore disappears from $\sum C_n f_n^2 - (\sum C_n f_n)^2$. We can therefore limit ourselves to the experimentally determined coherent nuclear cross section.¹⁵ From the preceding remarks it becomes apparent that the consideration of the crystalline structure of the material is decisive in any calculation of polarization effects. Not only does it allow us to take properly into account the coherent and incoherent contributions, but it is also, as previously remarked, essential in the introduction of the form factor for the magnetic scattering.

It would be permissible (cf. Section II and Fig. 1) to approximate the crystalline aggregate by an amorphous body for sufficiently small wave-length. But since the distribution of the magnetically active currents in an atom extends over a domain which is not small even compared with the wave-length of thermal neutrons, the case of small wave-length would become uninteresting, since the atomic form factor would almost annihilate the effect to be expected. Choosing, on the other hand, sufficiently large wave-lengths, we are no longer allowed to neglect the crystal structure. Coherent scattering disappears in the case of Fe for wave-lengths larger than 4.04Å. There does not therefore exist a range in which the theory based on an amorphous structure is even approximately correct.

A quantitative evaluation of polarization phenomena requires, therefore, knowledge of the wave-length of the incident neutrons, as well as of the form factor of the scattering atom which is a function of wave-length and scattering angle. We shall, in this section, assume, first, that

¹⁵ The background produced by inelastic collisions between the neutron and the lattice vibrations should, strictly speaking, also be considered. We neglect it in the following discussion because, it would be very small even for x-rays, still smaller for neutrons (cf. reference 4) and mostly present for large scattering angles, where its effect is strongly cut down by the form-factor.

¹⁴ See II and III.

monochromatic neutrons are incident, and discuss choice and influence of the form factor. Section VII contains the more general treatment of an incident spectrum together with a numerical evaluation of the results.

Polarization effects can be observed through experiments on the scattered or transmitted beam; only experiments of the second type have so far been performed, for reasons of available intensity. We shall therefore limit ourselves to this group of phenomena; the treatment of the scattered beams can easily be carried out with the aid of the formulae presented here and in previous notes.

As the incident beam is resolved along the direction of magnetization denoted by \mathbf{k} , the additional scattering per unit solid angle for the two spin states is given by¹⁶

$$d\Phi_{\text{additional}} = \pm 2CD(\mathbf{q} \cdot \mathbf{k})d\Omega = \pm 2CDq^2d\Omega. \quad (6.1)$$

This can be taken over to the crystalline case immediately since both the amplitudes C and D refer to coherent processes *only*. The magnetization is assumed to be perpendicular to the direction of incidence, as is the case in all experiments. In the crystalline case, for a ring of index $|l|$, the average of q^2 over azimuth gives

$$\langle q^2 \rangle_{\text{av}} = \frac{1}{2}(1 + \sin^2 \frac{1}{2}\theta) = \frac{1}{2}(1 + |l|^2\lambda^2/4a^2). \quad (6.2)$$

The form factor F which is contained in D is function of $|l|$ only. (From now on we shall write the form factor separately: $D = e^2\gamma S/mc^2$.)

The final result for the additional cross section p , for the case of a simple cubic crystal, including temperature effect, is:

$$\begin{aligned} p &= CD \cdot \frac{1}{2} \left(\frac{\lambda}{a}\right)^2 \sum_{|l| < 2a/\lambda} \frac{\exp(-A|l|^2)}{|l|} \\ &\quad \times F(|l|) \left(1 + \frac{|l|^2\lambda^2}{4a^2}\right) \\ &= 4\pi C^2 \cdot \frac{D}{C} \cdot \frac{1}{8\pi} \left(\frac{\lambda}{a}\right)^2 \sum_{|l| < 2a/\lambda} \frac{\exp(-A|l|^2)}{|l|} \\ &\quad \times F(|l|) \left(1 + \frac{|l|^2\lambda^2}{4a^2}\right) \end{aligned} \quad (6.3)$$

¹⁶ See III, Section VI. We here neglect small effects proportional to D^2 .

and comparing with

$$\bar{\sigma}_{\text{nuclear effective}} = \sigma \cdot \frac{1}{8\pi} \left(\frac{\lambda}{a}\right)^2 \sum_{|l| < 2a/\lambda} \frac{\exp(-A|l|^2)}{|l|}, \quad (2.15)$$

we obtain:

$$\begin{aligned} p &= \bar{\sigma}_{\text{nuc off}} \cdot \frac{D}{C} \\ &\quad \times \sum_{|l| < 2a/\lambda} f(|l|)F(|l|) \left(1 + \frac{|l|^2\lambda^2}{4a^2}\right), \end{aligned} \quad (6.4)$$

where $f(|l|)$ is the fraction of the scattered neutrons in the ring of index $|l|$.

The same formula will apply to any other case (average over velocity distribution; body-centered crystal). The “ p ” is always given by:

$$\bar{\sigma}_{\text{coherent}}(D/C) [\text{average over the rings of } F(|l|)(1 + |l|^2\lambda^2/4a^2)].$$

To find the additional scattering w for a centimeter thickness, we multiply by the number N of atoms/cc (for iron $N = 8.48 \times 10^{22}$); $w = Np$. Then the fractional increase in transmission on magnetization is:

$$\left(\frac{1}{2}e^{-N\sigma x - wx} + \frac{1}{2}e^{-N\sigma x + wx} - e^{-N\sigma x}\right)/e^{-N\sigma x}, \quad (6.5)$$

where σ contains the cross sections for all other causes of weakening of the beam (capture, incoherent scattering, nuclear coherent scattering), and x is the total thickness traversed. This gives for the fractional change in transmission

$$\frac{1}{2}w^2x^2. \quad (6.6)$$

This result applies to both single and double transmission experiments.

While the amplitude C of nuclear scattering is independent of the scattering angle, D will depend on it through the magnetic form factor. Its determination offers a certain difficulty due to our incomplete knowledge of the constitution of the magnetically active 3- d shell of Fe. For the purposes of a rough estimate we have previously¹⁷ used Slater's¹⁸ hydrogenic function for the wave function of the electrons in question. This method, which was also adopted with even

¹⁷ See Section VII of III.

¹⁸ J. C. Slater, Phys. Rev. **36**, 57 (1930).

steeper decrease towards the outside by Van Vleck,¹⁹ does not seem to lead to reliable quantitative values as successfully as it might have for other applications reported by Slater.

Bethe²⁰ used the well-tabulated density function of Hartree for the 3-*d* shell of Cu⁺, which was derived by the method of the self-consistent field. To adapt this density distribution to the case of iron with a smaller central charge, Bethe "expanded" the effective radius of iron with respect to copper in the inverse ratio of the effective charges and calculated the form factor by numerical integrations.

In the present paper we also use the Hartree distribution which has so far proved to be of higher accuracy than our demands would require. But in place of the slightly rough numerical integration carried out by Bethe, we use the analytic expression for the Hartree distribution as adapted by Slater.²¹ It is interesting to observe that the actual density distribution can be well represented by the sum of three hydrogenic functions of which only two are really significant. The result of this analytic calculation agrees with Bethe's formula for sufficiently small values of $(\sin\frac{1}{2}\theta)/\lambda$, but our probably more correct method gives a decidedly sharper decrease of the form factor at large angles.

For a Cu⁺ 3-*d* electron, the (radial density)^{1/2}

$$\sqrt{\rho} = r\psi = r^3(ae^{-br} + ce^{-dr} + fe^{-gr}).$$

The unit of length is the Bohr radius a_0 . $b = 6.29$; $d = 2.65$; $g = 1.28$. Slater gives the following data:

inner intersection = 3.78; i.e.,

$$ae^{-(3/3.78)(6.29)} = ce^{-(3/3.78)2.65}$$

and outer intersection = 1.15; i.e.,

$$ce^{-2.65(3/1.15)} = fe^{-1.28(3/1.15)}.$$

This gives $a = 17.975c$
 $f = 0.02804c$.

So we can write:

$$\sqrt{\rho} = r\psi = r^3[17.975e^{-6.29r} + e^{-2.65r} + 0.02804e^{-1.28r}].$$

¹⁹ J. H. Van Vleck, Phys. Rev. **55**, 924 (1939).

²⁰ Hoffman, Livingston and Bethe, Phys. Rev. **51**, 214 (1937).

²¹ J. C. Slater, Phys. Rev. **42**, 33 (1932).

To calculate the form factor, we must evaluate:

$$F = \int e^{i\rho r \cos\theta} \sin\theta d\theta \rho dr, \quad (6.7)$$

where $p = 2k \sin\frac{1}{2}\theta$; $k = 2\pi/\lambda$; λ in Bohr units. F will consist of six terms:

$$F = \sum_{i=1}^6 f_i$$

where f_i is of the form:

$$f_i = \int e^{i\rho r \cos\theta} \sin\theta d\theta \cdot l_i \exp(-m_i r) r^6 dr,$$

<i>i</i>	1	2	3	4	5	6
l_i	323.1	35.95	1.008	1.0	0.0561	0.00079
m_i	12.58	8.94	7.57	5.30	3.93	2.56

$$f_i = \frac{l_i}{i\rho} \int_0^\infty dr \cdot r^5 \exp(-m_i r) [e^{i\rho r} - e^{-i\rho r}]$$

$$= \frac{5l_i}{i\rho} \left[\frac{1}{(m_i - i\rho)^6} - \frac{1}{(m_i + i\rho)^6} \right]$$

$$= \frac{2 \cdot 6l_i}{m_i^7} \frac{1 - (10/3)(p/m_i)^2 + (p/m_i)^4}{[1 + (p/m_i)^2]^6}.$$

Normalization is obtained by requiring that for $p \rightarrow 0$, $F \rightarrow 1$. So we must divide by the normalization factor $\sum_1^6 2 \cdot 6l_i/m_i^7$. When this is done, we obtain the form factor: $F = \sum_1^6 F_i$, where

$$F_i = n_i \left[\frac{1 - (10/3)(p/m_i)^2 + (p/m_i)^4}{[1 + (p/m_i)^2]^6} \right]. \quad (6.8)$$

<i>i</i>	1	2	3	4	5	6
n_i	0.227	0.276	0.025	0.298	0.136	0.038
m_i	12.58	8.94	7.57	5.30	3.93	2.56

The form factor consists of these six terms, each similar to the single-term expression given in III. Figure 3 gives a comparison between F and the form factor F_B as given by Bethe. They coincide for small values of p , but F falls below F_B and decreases more rapidly for large p .

For a Debye-Scherrer ring of index $|l|$, $p = 2\pi a_0 |l|/d$. We see that F is a function only of $|l|$. For application to Fe, we have reduced the wave-length to 75 percent to take account of the contraction of the charge. The values of p for the first few rings are indicated in Fig. 3.

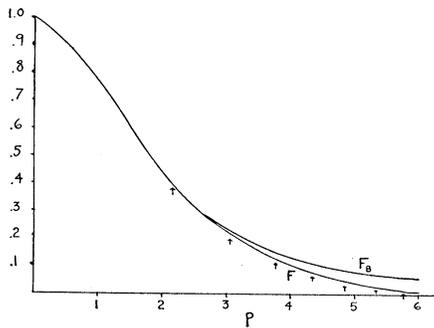


FIG. 3. Form-factor of 3d shell of iron.

VII. EVALUATION OF POLARIZATION EXPERIMENTS CONTINUED; VELOCITY DISTRIBUTION OF THE INCIDENT NEUTRONS

The strong dependence of the scattering into rings of different values of $|l|$ on the wavelength, as it becomes apparent from the formula (2.16) and from the discussion at the end of Section III, makes it necessary to refine the calculations of Section II, as far as the velocity distribution is concerned. It has been frequently observed that the Maxwellian distribution used in paragraph 2 for the purpose of illustration cannot really claim to be an accurate representation of the velocities present in the incident beam of "thermal neutrons." Neither are the long wave-lengths (small velocities) really present, since the inelastic transitions are far too slow to produce them (cf. Pomeranchuk⁵); nor can it be expected that the curve falls off at high velocities in an exponential manner, since the whole spectrum should extend even beyond the Cd absorption limit.

Absorption experiments with "cooled" neutrons also fail to show real agreement with the $1/v$ law, when temperatures of the neutron source are used for comparison.

We have therefore made use of the velocity curve which has been obtained by Dunning²² and collaborators giving the frequency of neutrons as a function of their mechanically determined speed. The result is contained in Fig. 4, where a Maxwell distribution has been included for comparison. (The distributions as shown are not normalized; their maxima have been made to

²² Dunning, Pegram, Fink, Mitchell and Segrè, Phys. Rev. **48**, 704 (1935).

coincide, in order to show clearly the difference in shape.) This choice brings with it the disadvantage of a numerical integration since no analytic representation of this velocity distribution is available. The velocity distribution shows qualitatively all the features to be expected.

A second point to be taken into account is the change in the velocity distribution while the neutrons pass through iron. The coherent scattering as well as the background are *approx-*

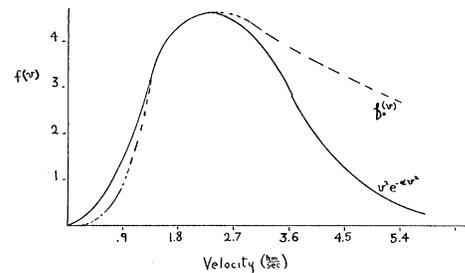


FIG. 4. Comparison of velocity-selector and Maxwellian distributions.

mately velocity independent; the capture on the other hand follows the $1/v$ law, and therefore removes the low velocity neutrons preferentially. Since it is the long wave-length, low velocity neutrons which determine the polarization, this correction will turn out to be of significance.

In order to determine the velocity distribution of the neutrons as a function of the thickness of sample traversed, we have proceeded as follows:

The observed capture cross section $\bar{\sigma}_{\text{cap}}$ of Fe for thermal neutrons is $\sim 3.5 \times 10^{-24}$ cm². This represents an average of the capture cross section $\sigma_{\text{cap}} = \sigma_0/v$ over the thermal distribution, i.e.,

$$\bar{\sigma}_{\text{cap}} = 3.5 \times 10^{-24} \text{ cm}^2 = \int \frac{\sigma_0}{v} f_0(v) dv / \int f_0(v) dv, \quad (7.1)$$

where $f_0(v)$ is the neutron distribution indicated in Fig. 4 and tabulated in Table I. This gives, after numerical integration,

$$\sigma_0 = 8.9 \times 10^{-19}; \quad \sigma_{\text{cap}} = \sigma_0/v. \quad (7.2)$$

The velocity distribution $f_x(v)$, after a thickness x has been traversed is given by:

$$f_x(v) = f_0(v) \exp(-N\sigma_0 x/v). \quad (7.3)$$

Using Eq. (7.3), the velocity distribution has

been calculated for thicknesses of 1, 2, 3 and 4 cm, and then a normalization factor introduced so that

$$\int_0^{5.4} f_x(v)dv = 1.$$

The function $f_x(v)$ is tabulated in Table I.

We must also replace the calculation of $\bar{\sigma}/\sigma$ given in Section III on the basis of Eq. (2.17), by a similar calculation using the correct neutron distribution $f_0(v)$. From Eq. (2.16) we obtain:

$$\bar{\sigma}/\sigma = \int_0^\infty f_0(v)dv \cdot \frac{2}{8\pi} \left(\frac{\lambda}{a}\right)^2 \times \sum_{\text{even } |l| < 2a/\lambda} \frac{\exp(-A|l|^2)}{|l|}, \quad (7.4)$$

where $f_0(v)$ has been assumed to be normalized. The order of summation and integration may be reversed, giving

$$\frac{\bar{\sigma}}{\sigma} = \sum_{\text{even } |l|} \frac{\exp(-A|l|^2)}{|l|} \cdot \frac{2}{8\pi} \left(\frac{h}{Ma}\right)^2 \times \int_{|l|h/2Ma}^\infty \frac{f_0(v)dv}{v^2}. \quad (7.5)$$

TABLE I. Values of $f_x(v)$.*

v (km./sec.)	$f_0(v)$	$f_1(v)$	$f_2(v)$	$f_3(v)$	$f_4(v)$
0.9	0.88	0.38	0.164	0.071	0.031
1.1	1.64	0.826	0.416	0.210	0.105
1.3	2.72	1.521	0.852	0.476	0.266
1.5	3.78	2.286	1.382	0.836	0.505
1.7	4.20	2.694	1.728	1.109	0.711
1.9	4.42	2.972	1.998	1.343	0.903
2.1	4.55	3.175	2.215	1.545	1.078
2.3	4.62	3.328	2.397	1.727	1.244
2.5	4.63	3.423	2.531	1.871	1.383
2.7	4.58	3.462	2.616	1.977	1.494
2.9	4.48	3.455	2.663	2.054	1.584
3.1	4.30	3.369	2.639	2.068	1.620
3.3	4.12	3.277	2.606	2.075	1.648
3.5	3.96	3.191	2.571	2.071	1.669
3.7	3.81	3.107	2.534	2.066	1.685
3.9	3.66	3.015	2.483	2.045	1.686
4.1	3.52	2.929	2.436	2.027	1.686
4.3	3.39	2.843	2.384	1.999	1.677
4.5	3.25	2.748	2.322	1.963	1.660
4.7	3.12	2.656	2.261	1.925	1.639
4.9	3.00	2.572	2.205	1.890	1.620
5.1	2.87	2.475	2.135	1.841	1.588
5.3	2.74	2.377	2.063	1.789	1.552
$\int_0^{5.4} f_x dv = 16.63$	12.408	9.562	7.284	5.256	

* More figures have been included in these tables than are physically significant. This has been done to assist the reader in following a sample calculation and in reproducing the graphs smoothly.

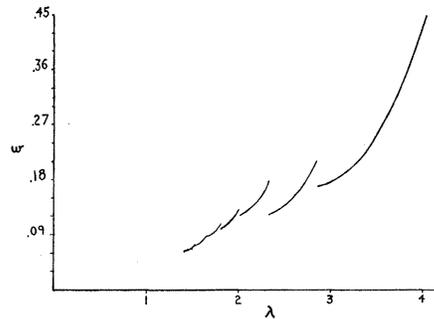


FIG. 5. Variation of polarization effect as a function of neutron wave-length.

From Eq. (7.5) we see that $\bar{\sigma}/\sigma$ consists of a sum of terms for different $|l|$, each involving a numerical integration of $f_0(v)/v^2$ from $v = |l|h/2Ma$ to ∞ . This has been carried out, giving $\bar{\sigma}/\sigma = 0.75$, which corresponds to $C = 7.33 \times 10^{-13}$ cm.

Using $\gamma = 1.93$;²⁴ $S = 1.07$, giving $D = e^2\gamma S/mc^2 = 5.8 \times 10^{-13}$, $N = 8.48 \times 10^{22}$, we have calculated w for monochromatic beams of various wave-lengths, using Eq. (6.4) and the ratio $\bar{\sigma}/\sigma$ given in Fig. 1.

The values of w obtained are shown in Fig. 5. The breaks in the curve occur at wave-lengths where a Debye-Scherrer ring is cut out, as has already been described in connection with Fig. 1.

For an incident beam of thermal neutrons, Eq. (6.6) will no longer apply, but will be replaced by

$$\frac{1}{2} \left[\int_0^d w(x)dx \right]^2 \quad (7.6)$$

for the transmission effect of a sample of thickness d ; we write $w(x)$ because the polarization will now vary with distance traversed, since the velocity distribution $f_x(v)$ is changing because of preferential absorption of low velocity neutrons.

To evaluate the polarization effect, we have calculated $w(x)$ for $x = 0, 1, 2, 3, 4$, cm using the values of $f_x(v)$ tabulated in Table I and using Eq. (6.4). The fraction $f^{(|l|)}$ is here given by the $|l|$ th term in Eq. (7.5), divided by the total value of that sum. The results are shown in Table II. It should be pointed out that the polarization factor $(1 + |l|^2\lambda^2/4a^2)$ depends on the wave-length. We have throughout used an

²⁴ L. W. Alvarez and F. Bloch, Phys. Rev. 57, 111 (1940).

TABLE II. Values of $w(x)$.*

$ \mu ^2$	$1 + \frac{A = \mu ^2 \lambda^2}{4a^2}$	$F(\mu)$	$f_0(v)$		$f_1(v)$		$f_2(v)$		$f_3(v)$		$f_4(v)$	
			$f(\mu)$	$fF(A)$								
2	1.14	0.39	0.281	0.125	0.252	0.112	0.231	0.103	0.207	0.092	0.193	0.086
4	1.29	.22	.076	.022	.071	.020	.068	.019	.063	.018	.061	.017
6	1.43	.13	.183	.034	.181	.034	.178	.033	.171	.032	.170	.032
8	1.57	.08	.061	.008	.062	.008	.062	.008	.061	.008	.062	.008
10	1.71	.047	.086	.0069	.089	.0071	.092	.0074	.092	.0074	.095	.0076
12	1.86	.027	.021	.0011	.022	.0011	.023	.0012	.023	.0012	.024	.0012
14	2.00	.013	.094	.0024	.098	.0025	.106	.0028	.109	.0028	.115	.0030
16	2.00	.010	.009	.0002	.010	.0002	.010	.0002	.011	.0002	.012	.0002
18	2.00	.008	.043	.0007	.046	.0007	.050	.0008	.052	.0008	.056	.0009
			Remainder	0.0004	0.0005		0.0004		0.0004		0.0005	
			Total =	.200	.186		.176		.163		.156	
			$w(x) =$.0676	.0627		.0588		.0549		.0529	

* More figures have been included in these tables than are physically significant. This has been done to assist the reader in following a sample calculation and in reproducing the graphs smoothly.

average value for $\lambda=1.53A$. This is justified since it is a slowly varying function of λ . Also, as the distribution changes while passing through the sample, the average wave-length decreases, so that, at worst, we are over-estimating the polarization effect.

We obtain from the data of Table II for the transmission effect the results shown in Table III where experimental results^{24,25} are listed for comparison:

TABLE III.

Thickness	0.8	1.3	1.95	4.0
% Effect	0.14	0.35	0.75	2.9
Experimental	0.76	1.78	3.32	6.0

As can be seen from the table, there exists a considerable discrepancy between theoretical and observed values for the transmission. We have also, in our comparison, to take into account

the marked depolarization effect due to deviation from saturation.² The data given by the experimenters do not allow us to draw any very definite conclusion about the state of saturation obtained, and we shall therefore defer the more detailed discussion of that effect until later. The presence of the depolarization effect is clearly indicated by the marked deviation from the law:

$$\text{polarization effect} \propto (\text{thickness})^2.$$

We do not, at the moment, see any possibility of reconciling the observed data with the present accepted views about the magnetic interaction between neutron and iron atom, and the constitution of the iron crystals. We intend to return to a fuller discussion of the questions involved in this field in a later paper.²⁶

²⁵ P. N. Powers, Phys. Rev. **54**, 827 (1938).

²⁶ O. Halpern and M. H. Johnson, Phys. Rev. **57**, 160 (1940).