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The Effect of Crystal Orientation on the Scattering of Slow Neutrons

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Introduction

The transmission of slow neutrons through microcrystalline materials has been the subject of several investigations.[1,2,3] However, the effect of non-random orientations of the microcrystals on neutron scattering has not been considered in detail. We shall develop a simplified scheme for taking account of the orientation effect when only a single symmetry axis needs to be considered. A comparison is made with the measurements of the transmission of slow neutrons through randomly oriented and extruded graphite. It is possible to obtain an estimate of the amount of crystal orientation in this instance.

Theory

Let us call ψ the angle between the direction of extrusion and the axis of symmetry of a given crystal. The probability of finding a crystal oriented in the solid angle $d(\cos\psi)\,d\omega$ will be taken to be

$$P(\cos\psi)\, d(\cos\psi)\, d\omega. \qquad (1)$$

Let $\vec{b}$ denote product of the order of the Bragg reflection and the reciprocal lattice vector. The symmetry axis of the crystal will be in the direction of one of the basic reciprocal lattice vectors, for example, $\vec{b}_3$.

$$\vec{b} = \ell\vec{b}_1 + m\vec{b}_2 + n\vec{b}_3. \qquad (2)$$

1. O. Halpern, M. Hammermesh, and M. H. Johnson, Phys. Rev. <u>59</u>, 981 (1941).
2. R. Weinstock, Phys. Rev. <u>65</u>, 1 (1944).
3. E. Fermi, W. Sturm, and R. Sachs, Phys. Rev. <u>71</u>, 589 (1947).

ℓ, m, n are the products of the order of the reflection and the Miller indices leading to the particular Bragg reflection under consideration.

A. Incident Neutron Beam Parallel to Extrusion Direction.

The details are depicted in Fig. 1. The scattering for a particular Bragg reflection into the solid angle $d(\cos\psi)\,d\omega$ is[3]

$$\sigma_b\, d(\cos\psi)d\omega = \frac{FN\lambda^2}{2\pi b^2\Delta\lambda}\exp(-wb^2)\,P(\cos\psi)\,d(\cos\psi)\,d\omega \qquad (3)$$

F is the form factor for the unit cell in the crystal, N is the number of unit cells per unit volume, and $\Delta\lambda$ gives the spread in the wave-length of the incident neutron beam, $\exp(-wb^2)$ is the factor which takes into account the zero point and thermal oscillations of the crystal, w being a function of the Debye temperature and temperature of the lattice.[2]

Transforming to the variables θ, ϕ it is easily shown that

$$\begin{aligned}\cos\psi &= \cos\theta\cos\alpha + \sin\theta\sin\alpha\cos\phi \\ &= \frac{nb_3}{b}\cos\theta + \left(1 - \frac{n^2b_3^2}{b^2}\right)^{\frac{1}{2}}\sin\theta\cos\phi \end{aligned} \qquad (4)$$

and $d(\cos\psi)d\omega = d(\cos\theta)d\phi$.

Making use of the Bragg relation $\cos\theta = \frac{b\lambda}{2}$ and treating $\Delta\lambda$ as small, there results;

$$\int \sigma_b d(\cos\psi)d\omega = \frac{FN\lambda^2}{4\pi b}\exp(-wb^2)\int_0^{2\pi} P(\theta,\phi)d\phi \qquad (5)$$

In order to proceed further, it is necessary to make some specific assumptions about the nature of the function $P(\cos\psi)$. We will consider a distribution function with two parameters, namely

$$P = \frac{1}{4\pi} + x(\cos^2\psi - 1/3) + y(\cos^4\psi - 1/5). \qquad (6)$$

The quantities x and y give a measure of the degree of correlation in orientation between the crystals, and they are subject to the limitation that P shall remain positive for all values of ψ. The factors 1/3 and 1/5 are necessary in (6) in order that which corresponds to random orientation. Substituting the above expression for P in Eq. (5), we have

$$
\begin{aligned}
\int \sigma_d(\cos\psi)\,d\omega = \frac{FN\lambda^2}{4\pi b} \exp(-wb^2) \Big\{ & \left(\tfrac{1}{2} - \frac{2\pi x}{3} - \frac{2\pi y}{5}\right) \\
& + 2\pi x \left[\frac{b^2\lambda^2}{4} \cdot \frac{n^2 b_3^2}{b^2} + \tfrac{1}{2}\left(1 - \frac{b^2\lambda^2}{4}\right)\left(1 - \frac{n^2 b_3^2}{b^2}\right) \right] \\
& + 2\pi y \left[\frac{b^4\lambda^4}{16} \, \frac{n^4 b_3^4}{b^4} + 3\, \frac{b^2\lambda^2}{4}\left(1 - \frac{b^2\lambda^2}{4}\right)\left(\frac{n^2 b_3^2}{b^2}\right)\left(1 - \frac{n^2 b_3^2}{b^2}\right) \right. \\
& \left. + 3/8 \left(1 - \frac{b^2\lambda^2}{4}\right)^2 \left(1 - \frac{n^2 b_3^2}{b^2}\right)^2 \right] \Big\}
\end{aligned}
\tag{7}
$$

(7) must now be summed over all planes which satisfy the Bragg condition. Transforming from neutron wave-length to energy,

$$
\begin{aligned}
\sigma_c = \sum_{E_b \le E}{}' \frac{FNE_b}{2\, b^3 E} \exp(-wb^2) \Big\{ & \left(1 - \frac{4\pi x}{3} - \frac{4\pi y}{5}\right) \\
& + 4\pi x \left[\frac{E_b}{E} \cdot \frac{n^2 b_3^2}{b^2} + \tfrac{1}{2}\left(1 - \frac{E_b}{E}\right)\left(1 - \frac{n^2 b_3^2}{b^2}\right) \right] \\
& + 4\pi y \left[\frac{E_b^2}{E^2} \cdot \frac{n^4 b_3^4}{b^4} + 3\, \frac{E_b}{E}\left(1 - \frac{E_b}{E}\right)\left(\frac{n^2 b_3^2}{b^2}\right)\left(1 - \frac{n^2 b_3^2}{b^2}\right) \right. \\
& \left. + 3/8 \left(1 - \frac{E_b}{E}\right)^2 \left(1 - \frac{n^2 b_3^2}{b^2}\right)^2 \right] \Big\}
\end{aligned}
\tag{8}
$$

σ_c is the coherent scattering cross section at the neutron energy E; E_b is the neutron energy at a particular Bragg limit.

B. Incident Neutron Beam Perpendicular to Extrusion Direction.

If the incident neutron beam is perpendicular to the direction of extrusion, the previous analysis must be modified slightly. We need merely to rotate the direction of the incident beam through 90°. We have as before

$$\cos\psi = \frac{nb_3}{b}\cos\theta' + \left(1 - \frac{n^2 b_3^2}{b^2}\right)^{\frac{1}{2}} \sin\theta' \cos\phi$$

with $\theta' = \theta - 90^{\circ}$.

In this instance,

$$\sigma_c = \sum_{E_b \leq E} \frac{FNE_b}{2\pi b^3 E} \exp(-wb^2) \left\{ \left(1 - \frac{4\pi x}{3} - \frac{4\pi y}{5}\right) \right.$$

$$+ 4\pi x \left[\left(1 - \frac{E_b}{E}\right) \frac{n^2 b_3^2}{b^2} + \frac{1}{2}\frac{E_b}{E}\left(1 - \frac{n^2 b_3^2}{b^2}\right) \right] \qquad (9)$$

$$+ 4\pi y \left[\left(1 - \frac{E_b}{E}\right)^2 \frac{n^4 b_3^4}{b^4} + 3\frac{E_b}{E}\left(1 - \frac{E_b}{E}\right)\left(\frac{n^2 b_3^2}{b^2}\right)\left(1 - \frac{n^2 b_3^2}{b^2}\right) \right.$$

$$\left. \left. + \frac{3}{8}\frac{E_b^2}{E^2}\left(1 - \frac{n^2 b_3^2}{b^2}\right)^2 \right] \right\}$$

Cross Sections for Graphite

A mechanical velocity selector in conjunction with the heavy water pile at the Argonne Laboratory has been used to measure the cross sections for randomly oriented and extruded graphite.[4] In the computation of the theoretical curves, a free atom cross section of 4.5 barns was used, and the Debye temperature of graphite was taken to be 1569°K. The theoretical curve for the powdered graphite (random orientation) is, of course, the one corresponding to $x = y = 0$. In the case of the extruded material, the theoretical curves are fairly sensitive to the choice of the parameters x and y. The following values of these constants yielded about the best agreement with the empirical data:

$$x = -0.07, \; y = 0.04.$$

The results are shown in Fig. 2 - 4; the theoretical curves for the extruded material were calculated using the above constants. The agreement with

4. A. H. Weber, Fifth Annual Pittsburgh Conference on X-Ray and Electron Diffraction.

experiment is seen to be fairly satisfactory. The rise in the experimental curves below the first Bragg limit is probably due to a considerable amount of inelastic scattering.

The orientation function is

$$\begin{aligned} P &= 1/4\pi - 0.07\,(\cos^2\psi - 1/3) + 0.04\,(\cos^4\psi - 1/5) \\ &\simeq 1/4\pi\,(1.2 - 0.9\cos^2\psi + 0.5\cos^4\psi). \end{aligned} \quad (11)$$

It is seen that $P(\cos\psi = 1) < P(\cos\psi = 0)$. This means that the six-fold symmetry axis of graphite tends to be perpendicular to the direction of extrusion so that the hexagonal planes show a preferential alignment along the extrusion direction.

This report is based on work done under the auspices of the Atomic Energy Commission at the Argonne National Laboratory.

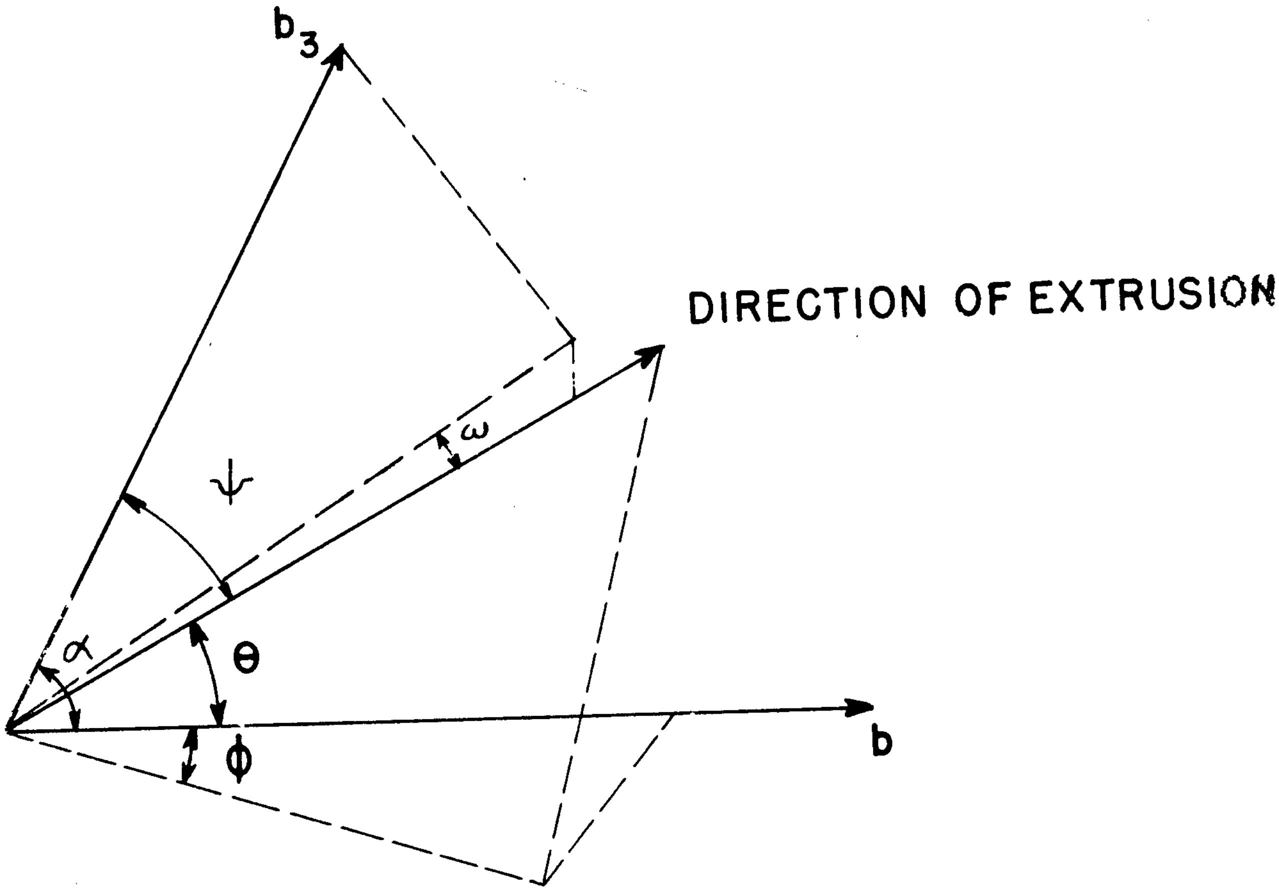


FIG. I

Fig. 1 Angles used in calculating the orientation effect. The azimuth ϕ is measured with respect to a plane passing through $\vec{b}$ and $\vec{b_3}$. The azimuth ω gives the projection of $\vec{b_3}$ relative to a plane passing through the extrusion direction.

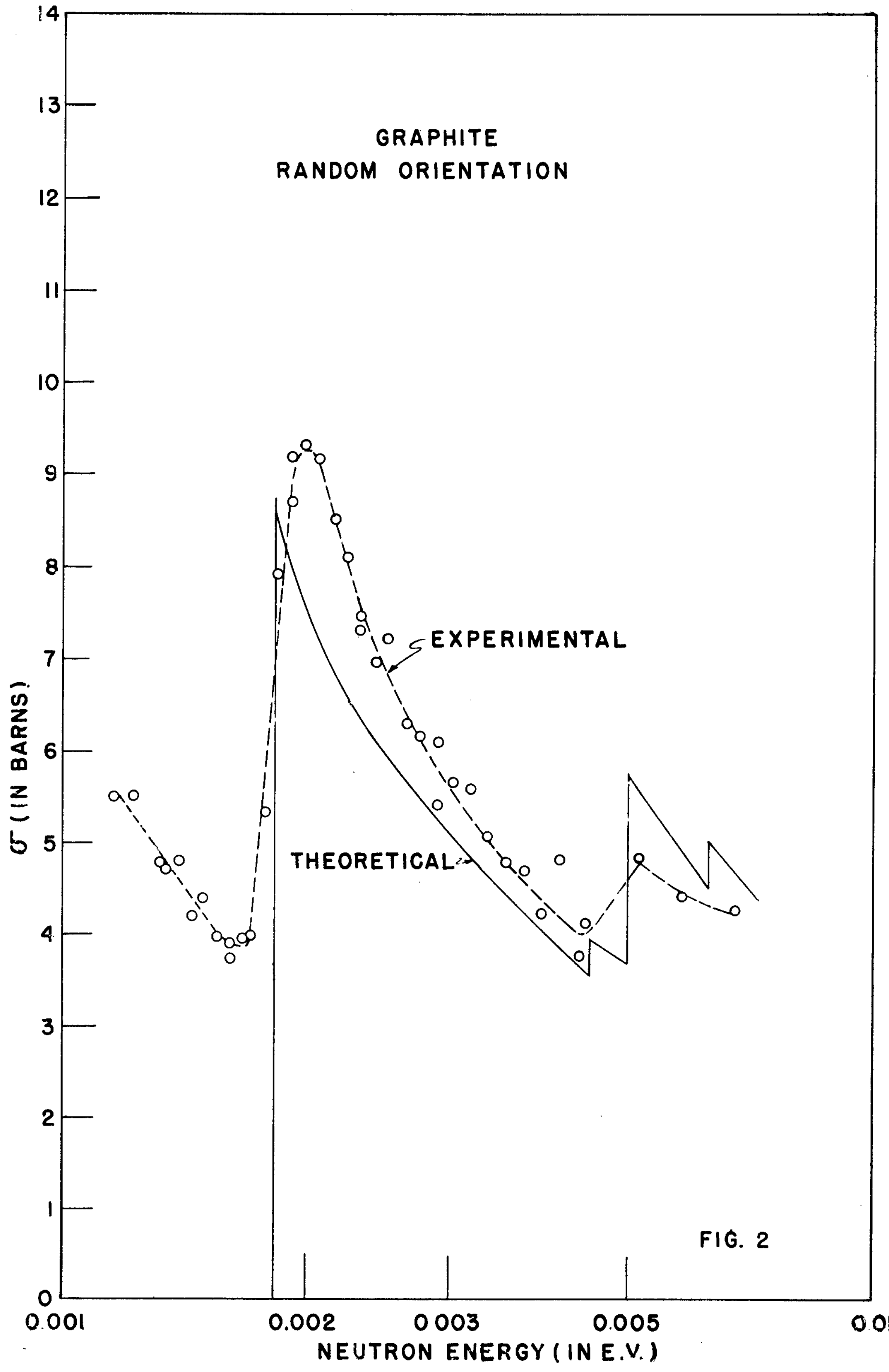
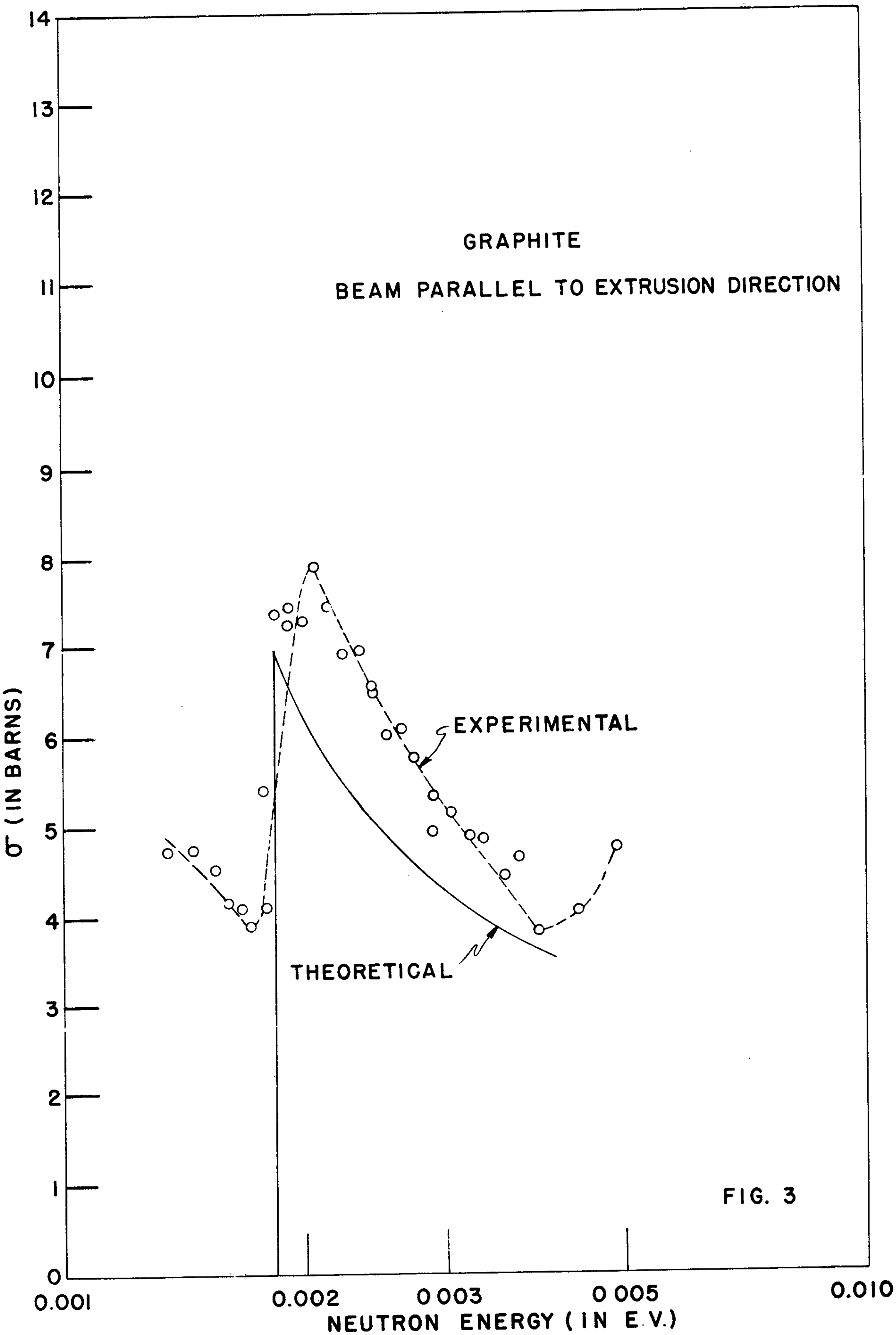

GRAPHITE
RANDOM ORIENTATION
EXPERIMENTAL
THEORETICAL
σ (IN BARNS)
NEUTRON ENERGY (IN E.V.)
0
1
2
3
4
5
6
7
8
9
10
11
12
13
14
0.001
0.002
0.003
0.005
0.01

FIG. 2


GRAPHITE
BEAM PARALLEL TO EXTRUSION DIRECTION
EXPERIMENTAL
THEORETICAL
σ (IN BARNS)
NEUTRON ENERGY (IN E.V.)
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3
4
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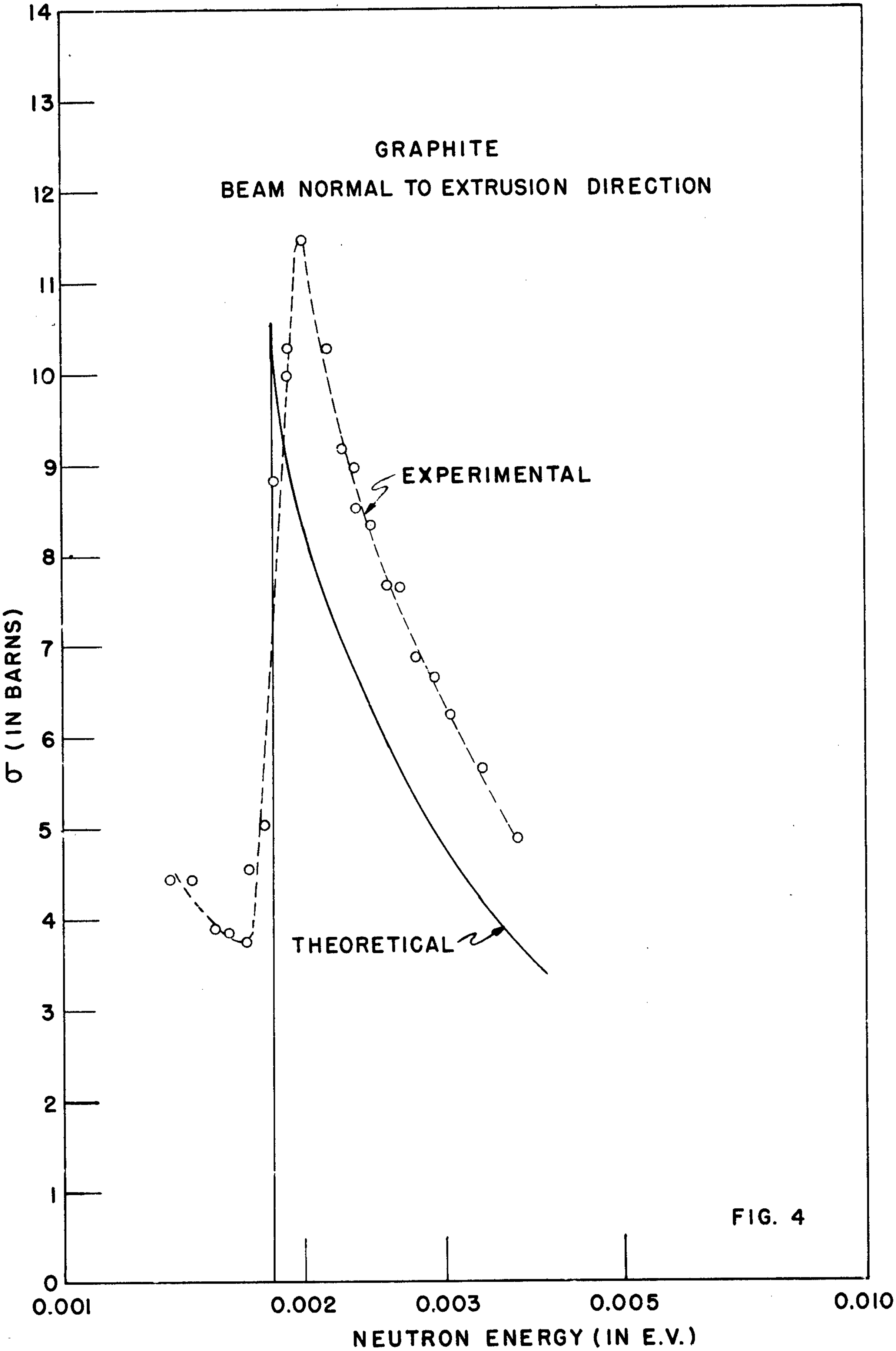
0.001
0.002
0.003
0.005
0.010

FIG. 3


GRAPHITE
BEAM NORMAL TO EXTRUSION DIRECTION
EXPERIMENTAL
THEORETICAL
σ (IN BARNS)
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0
0.001
0.002
0.003
0.005
0.010
NEUTRON ENERGY (IN E.V.)

FIG. 4