domain the average contribution will be J_s, as before, but for the layer on the extreme right of each domain F and F^* belong to *adjacent* domains, and the average contribution will be

$$J_a \equiv \langle F'F^* \rangle , \quad (6)$$

where the prime indicates that F and F' are the values of the structure factors of adjacent domains. If the total number of layers is N and the number of domain boundaries is K,

$$J(1) = N^{-1}[(N-K)J_s+KJ_a] , \quad (7)$$

it being assumed that N and K are so large that end effects can be neglected. On rearranging and putting $K/N = \lambda$, this becomes

$$J(1) = J_s-\lambda(J_s-J_a) . \quad (8)$$

For $t = 2$ the average contribution of each layer to $J(t)$ will be J_s for the $N-2K$ layers (approximately; the approximation consists in neglecting single-layer domains) for which F and F^* belong to the same domain, and J_a for the $2K$ layers (approximately) for which they belong to adjacent domains. The value of $J(t)$ is thus

$$J(2) \sim N^{-1}[(N-2K)J_s+2KJ_a] = J_s-2\lambda(J_s-J_a) , \quad (9)$$

and, in general, for small t,

$$J(t) \sim J_s-t\lambda(J_s-J_a) . \quad (10)$$

Now J_s is positive, from its definition. J_a is ordinarily negative—in a simple case (Wilson, 1949, p. 49) it is equal to $-J_s$ —but it cannot be greater in absolute value than J_s. For small t, therefore, $J(t)$ must decrease linearly with $|t|$, and thus has a cusp at the origin, like the Laplacian form, whatever the distribution function $p(\varepsilon)$. A similar argument for a cusp at the origin of $J(t)$ was given by MacGillavry & Strijk. The observed rounded origin must therefore be attributed either to a defect in the model of ordered domains separated by boundaries, or to experimental errors. One of the latter not explicitly discussed by Steeple & Edmunds (1956) is the estimation of the background level.

References

EASTABROOK, J. N. & WILSON, A. J. C. (1952). *Proc. Phys. Soc.* B, **65**, 67.
EDMUNDS, I. G. & HINDE, R. M. (1952). *Proc. Phys. Soc.* B, **65**, 716.
LANDAU, L. (1937). *Phys. Z. Sowjet.* **12**, 579.
LIFSCHITZ, I. M. (1937). *Phys. Z. Sowjet.* **12**, 623.
MACGILLAVRY, C. H. & STRIJK, B. (1946). *Physica*, **12**, 129.
STEEPLE, H. & EDMUNDS, I. G. (1956). *Acta Cryst.* **9**, 934.
STOKES, A. R. (1948). *Proc. Phys. Soc.* **61**, 382.
STRIJK, B. & MACGILLAVRY, C. H. (1946). *Physica*, **11**, 369.
WILSON, A. J. C. (1942). *Proc. Roy. Soc.* A, **180**, 277.
WILSON, A. J. C. (1943). *Proc. Roy. Soc.* A, **181**, 360.
WILSON, A. J. C. (1949). *X-ray Optics*. London: Methuen.

Acta Cryst. (1958). **11**, 228

The scattering of 4 Å neutrons by a beryllium crystal.

By H. J. HAY, N. J. PATTENDEN and P. A. EGELSTAFF, *Atomic Energy Research Establishment, Harwell, England*

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Analysis of the reflexions of X-rays from beryllium has shown that the crystal has the hexagonal close-packed lattice with $c = 3{\cdot}58$ Å and $a = 2{\cdot}29$ Å (Gordon, 1949). Measurements of the energies of Bragg-reflected neutrons from a single beryllium crystal, used as monochromator on a neutron spectrometer (Pattenden & Baston, 1957), have shown appreciable intensities of low-energy neutrons which would not be expected if the crystal has the above structure. There appear to be first-order reflexions from (0001) and (11$\bar{2}$1) planes, members of a class of planes which should have a zero atomic structure factor. Quantitative agreement between three different crystals suggested that the phenomenon might be a general property of beryllium crystals.

In order to verify that the effect was genuine, the following decisive experiment was performed.

A beryllium crystal, $1\frac{1}{4}$ in.$\times 1\frac{1}{4}$ in.$\times \frac{1}{4}$ in., was placed in a beryllium-filtered cold neutron beam containing a negligible number of neutrons with wavelengths shorter than 3·95 Å (Egelstaff & Pease, 1954; Butterworth *et al.*, 1957). Any Bragg reflexion, if observed, could be due to only the (0001) planes. Neutrons scattered through an angle of 73° from the beam were counted, corresponding to wavelengths of 4·26 Å for (0001) and 2·13 Å for (0002) Bragg reflexions. The arrangement is shown in Fig. 1. The results of a rocking-curve measurement are plotted

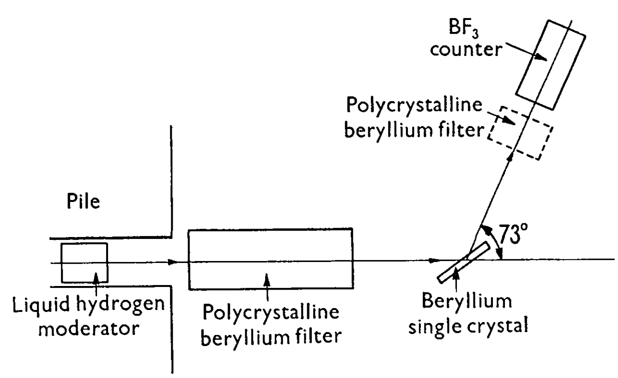

Fig. 1. Experimental arrangement.

in Fig. 2, and show an (elastically) scattered peak superimposed on a background of (inelastically) scattered neutrons. This interpretation was confirmed by placing a polycrystalline beryllium block in front of the detector.

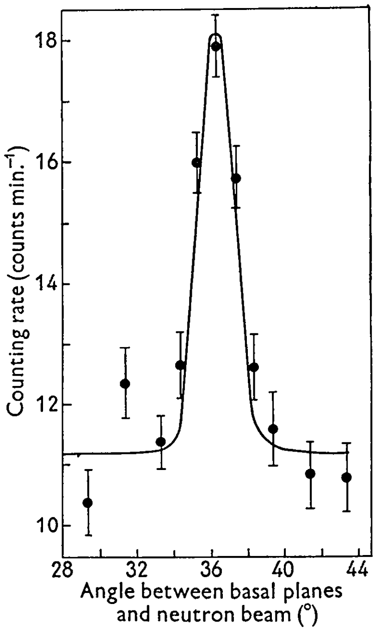

Fig. 2. Rocking curve for Be crystal. Counter at 73° from the neutron beam. The plotted points are for the cold neutron beam, and the curve is the (0002) Bragg reflexion at 2·13 Å (normalized to this ordinate scale).

The count rate of the peak was attenuated to 50% of its previous value, showing that it consisted of neutrons with wavelengths greater than 4 Å; the background count rate decreased to 3%, as expected if it consisted of (accelerated) inelastically scattered neutrons.

The 4 Å peak occurred at the same angle and, after subtraction of the background, had the same shape and position as a Bragg reflexion from the (0002) planes. The rocking curve for the latter reflexion was made with the beryllium filter removed from the incident beam.

When the crystal temperature was raised to 300° C., the measured peak counting rate was $0{\cdot}96 \pm 0{\cdot}20$ relative to the rate at room temperature. The inelastic scattering increased fourfold, which is in accordance with the variation of the inelastic cross-section with temperature. The room-temperature differential cross-section for inelastic scattering has been calculated to be 27 millibarns/steradian at an angle of 73° (Egelstaff, 1953), so that the elastic scattering cross-section can be deduced from the observed ratio of counting rates for elastic and inelastic scattering. Because of uncertainties in the absolute value of the calculated inelastic cross-section, in the spectral distributions of the incident and scattered neutrons, and in the counter efficiency, we consider that the estimated cross-section may be in error by up to a factor five. With this limitation, the cross-section for Bragg scattering at 4·26 Å is 0·6 millibarns.

There are a variety of possible explanations for the original and the present observations. We list six below:

(*a*) The occurrence of multiple Bragg reflexions.
(*b*) Reflexions occur from impurities, such as BeO, in the crystal.
(*c*) The structure of Be is not truly hexagonal close packed.
(*d*) Beryllium is antiferromagnetic.
(*e*) There is nuclear alignment and nuclear antiferromagnetism.
(*f*) Quasi-elastic peaks occur in the angular distribution of inelastically scattered neutrons.

Explanations (*d*), (*e*) and (*f*) are valid only for neutrons. Items (*a*) and (*b*) have been ruled out on the basis of a study of the energies and positions of various Bragg reflexions (of neutrons) by beryllium (Hay & Pattenden, 1958); (*a*) is also ruled out by the present work. Items (*d*), (*e*) and (*f*) are improbable on theoretical grounds. In particular, the observed temperature independence is probably inconsistent with (*f*).

If possibility (*c*) is correct, then the additional reflexions should be seen by X-rays as well as neutrons. No mention of them is made in the literature, although X-ray reflexions which cannot be indexed have been reported (e.g. Sidhu & Henry (1950), and references by Gordon (1949), Seybolt, Lukesh & White (1951)). To investigate this point further, a search for a (0001) reflexion was made on the same crystal, using Mo K X-radiation ($\lambda = 0{\cdot}7$ Å), but it failed to detect any reflexion having an intensity above the background scattering recorded on the X-ray film. This implies that, if the reflexion were present, it was considerably less than 1% of the observed (0002) reflexion. The absence of an X-ray reflexion would rule out (*b*) and (*c*), and possibly (*a*), and make (*d*), (*e*) or (*f*) probable.

We conclude that the observed phenomenon was coherent Bragg scattering of neutrons from the (0001) planes in beryllium, and that the explanation is obscure. We suggested that more information could profitably be obtained by further experimental work in two directions: (i) a more careful X-ray study; (ii) higher-energy neutron work, using time-of-flight methods. A deeper theoretical investigation of the 'improbable' explanations would be worthwhile.

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References

Butterworth, I., Egelstaff, P. A., London, H. & Webb, F. J. (1957). *Phil. Mag.* (8), **2**, 917.

Egelstaff, P. A. (1953). A. E. R. E. Report N/R 1164.

Egelstaff, P. A. & Pease, R. S. (1954). *J. Sci. Instrum.* **31**, 207.

Gordon, P. (1949). *J. Appl. Phys.* **20**, 908.

Hay, H. J. & Pattenden, N. J. (1958). To be published.

Pattenden, N. J. & Baston, A. H. (1957). A. E. R. E. Report NP/R 2251.

Seybolt, A. U., Lukesh, J. S. & White, D. W. (1951). *J. Appl. Phys.* **22**, 986.

Sidhu, S. S. & Henry, C. O. (1950). *J. Appl. Phys.* **21**, 1036.