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A geometrical consideration in the design of neutron spectrometers.

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Willis (1960) has shown, from the geometry of the double-crystal spectrometer, that the resolution of high-angle neutron-diffraction lines is greatly improved by reflecting the reactor beam from the monochromator crystal at a relatively high Bragg angle.

In this communication it is shown that a further gain in resolution can be obtained by choosing a suitable value for the ratio between the source-to-monochromator distance, and the monochromator-to-specimen distance.

This focusing effect can be illustrated by considering the path of the extreme rays in the collimator and their divergence after diffraction from the edges of the specimen. The assumption is made that the monochromator is operating under severe extinction conditions so that its reflectivity is effectively constant over the angular range of the incident neutrons.

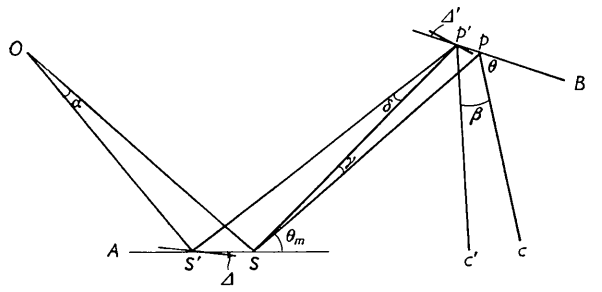

Fig. 1. General path of a neutron through the spectrometer.

The path of the neutron through the spectrometer is shown in Fig. 1. *OSPC* is the ray which passes down the collimator axis and is reflected at an angle θ_m by the plane of mean orientation in the monochromator A and at an angle θ by the mean plane in the specimen B; $OS'P'C'$ is a ray which is incident on A at $\theta_m+\alpha$ and is reflected to C' by the planes of orientation Δ and Δ' in A and B. Let us put $\angle PSP'=\gamma$ and $\angle S'P'S=\delta$, and choose the signs of α, Δ, Δ' and γ so that the glancing angles of the neutrons on A and B are increased if they are positive. δ always has the same sign as α.

The neutrons incident on B along $S'P'$ are reflected from A by the planes of orientation

$$\Delta=-\tfrac{1}{2}(\alpha+\delta-\gamma)\,.$$

The Bragg angle for reflection from these planes is

$$\theta_m+\alpha+\Delta=\theta_m+\tfrac{1}{2}(\alpha-\delta+\gamma)$$

so that the fractional difference in wavelength between neutrons incident on P and P' is

$$\Delta\lambda/\lambda=\tfrac{1}{2}(\alpha-\delta+\gamma)\cot\theta_m\,. \qquad (1)$$

It can be seen from this equation that for $\delta=\alpha$ the wavelengths of neutrons incident at any point P' on the specimen are the same.

Powder spectrometer

The difference in Bragg angle for neutrons incident on P and P' is

$$\Delta\theta=(\Delta\lambda/\lambda)\tan\theta$$
$$=(m/2)(\alpha+\gamma-\delta) \text{ from (1)}$$

where

$$m=\tan\theta/\tan\theta_m\,.$$

The divergence of the ray $P'C'$ from PC is then, for the parallel arrangement of the spectrometer,

$$\beta(2\theta)=2\Delta\theta-\gamma+\delta$$
$$=m(\alpha+\gamma-\delta)-\gamma+\delta\,.$$

Writing $k=\delta/\alpha$ this becomes

$$\beta(2\theta)=m\alpha(1-k)+\gamma(m-1)+k\alpha\,. \qquad (2)$$

For the extreme rays the following equations can be written down from (2):

$$\beta(2\theta)=m\alpha_m(1-k)+\gamma_m(m-1)+k\alpha_m$$
$$\beta(2\theta)=m\alpha_m(k-1)+\gamma_m(m-1)-k\alpha_m$$
$$\beta(2\theta)=m\alpha_m(1-k)+\gamma_m(1-m)+k\alpha_m$$
$$\beta(2\theta)=m\alpha_m(k-1)+\gamma_m(1-m)-k\alpha_m$$

where α_m and γ_m are the maximum numerical values of α and γ. For any particular spectrometer geometry (k) or spectrometer setting (m) the member of this set

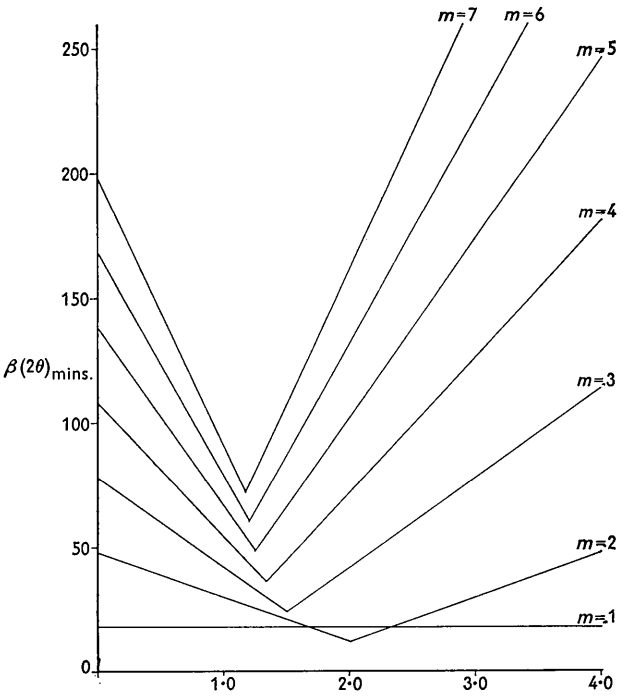

Fig. 2. The variation with m and k of the maximum divergence of the beams diffracted from a powder specimen.

of equations giving the maximum value of $\beta(2\theta)$ is the expression for the maximum divergence of the twice-reflected beam. In Fig. 2 this maximum value of $\beta(2\theta)$ has been plotted against k for various values of m. α_{max} has been taken as 18 minutes and γ_{max} as 12 minutes which are typical figures for the HIFAR powder-spectrometer assembly.

Single-crystal spectrometer

For diffraction from single crystals the natural width of the diffracted beam is the angle through which the crystal can be rotated from the position of maximum count rate and still reflect neutrons into the counter.

The mosaic distribution in crystal B is taken as

$$W(\Delta') = \text{const for } \Delta' \leq \eta$$
$$W(\Delta') = 0 \qquad \text{for } \Delta' > \eta$$

where η is the normal mosaic spread parameter. The angle $\beta(\theta)$ over which the crystal will reflect can then be written down from Fig. 1 as

$$\beta(\theta) = 2\Delta' - \gamma + \delta + \Delta\theta$$

which gives

$$\beta(\theta) = (\gamma/2)(m-2) + (\alpha/2)(m(k-1) - 2k) + 2\Delta'.$$

The appropriate maximum value of $\beta(\theta)$ is then chosen from

$$\begin{aligned}\beta(\theta)_{max} &= (\gamma_m/2)(m-2) + (\alpha_m/2)[m(k-1) - 2k] + 2\eta \\ &= (\gamma_m/2)(m-2) - (\alpha_m/2)[m(k-1) - 2k] + 2\eta \\ &= (\gamma_m/2)(2-m) + (\alpha_m/2)[m(k-1) - 2k] + 2\eta \\ &= (\gamma_m/2)(2-m) - (\alpha_m/2)[m(k-1) - 2k] + 2\eta\,.\end{aligned}$$

$\beta(\theta)_{max}$ has minima at $m=2$ and $m=2k/(k-1)$, so that for optimum resolution $k \to 1$ as $m \to \infty$.

In practice the sharp minima will be smeared out by the effects of a finite neutron source and reflection at finite depths in the monochromator crystal; however the gain in resolution given by working with $k \sim 1{\cdot}5$ should be evident over the range of m usually used.

Reference

WILLIS, B. T. M. (1960). *Acta Cryst.* **13**, 763.

Book Reviews

***Works intended for notice in this column should be sent direct to the Editor** (A. J. C. Wilson, Department of Physics, University College, Cathays Park, Cardiff, Great Britain). As far as practicable books will be reviewed in a country different from that of publication.*

General Catalogue of UNESCO Publications and UNESCO Sponsored Publications, 1946–1959. Pp. xvi+217. Paris: UNESCO, 1962. Price $1·00, 5/–, or 3·50 NF.

This bound volume contains particulars of 2681 books, arranged in accordance with the universal decimal classification, which have been published by or with the assistance of UNESCO. There is also the list of film strips and art slides occupying about six pages, a general index of forty pages, giving titles and authors, and a list of publishers with addresses. Explanatory matter is given in both French and English, and titles are given mostly in the language of the publication, though those in oriental languages are usually in English (occasionally French).

This publication will be extremely useful, but it leaves a good deal to be desired. Those publications of the International Union of Crystallography which were subsidized by UNESCO appear under the heading 'Mineralogical Sciences', and in fact there is only one other publication under this heading, a report of a conference held by the International Union of Pure and Applied Physics on defects in crystalline solids. A casual look through has revealed several misprints such as 'Bad rabit' and an error in the dollar price of *Current Sociology*. There are several abbreviations, presumably well recognized in the book-selling trade, but unintelligible to the general reader. The Index of Manufacturers of Apparatus and Materials used in Crystallography is described as 'S.I., s.n., s.d.', and these initials do not appear to be explained anywhere. However, the usefulness of the publication will outweigh these minor defects, and it is stated that a second corrected edition will be published in due course.

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Encyclopaedic Dictionary of Physics. Edited by J. THEWLIS. Volume 2, pp. ix+880. Volume 3, pp. ix+894. Volume 4, pp. ix+836. Volume 5, pp. ix+782. Oxford: Pergamon Press. Price £106 for the complete set [number of volumes not stated].

Volume 5 ends with 'Radiation constants', so this series of impressive volumes must be coming near its end. Volume 1 has been reviewed in some detail (*Acta Cryst.*, **15**, 626), and a briefer description of the current four will suffice.

There are many articles of great interest to crystallographers. For example, over twenty pages are devoted to counters of one type or another, and two pages of these are devoted to counting statistics, a subject not always as familiar as it should be. Diffractometers, on the other hand, get eight lines, with no cross-references. The entry 'Diffuse reflection, thermal' has nothing to do with X-ray diffraction. The article on diffraction analysis has a rather old-fashioned flavour, and is, perhaps significantly, unsigned. The treatments of electron diffraction and neutron diffraction are reasonably complete, given the necessary limitation of space in a