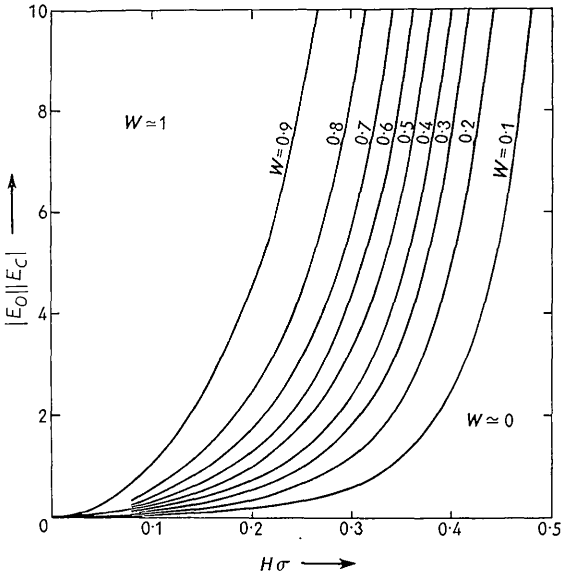

Fig. 1. Weighting function W plotted against $|E_o||E_c|$ and $H\sigma$.

equation (25) of Vand & Pepinsky the equation of the boundary at which $W=\frac{1}{2}$ is given in the non-centrosymmetric case by

$$|E_c||E_o| = 1.15 \sinh u^2,$$

which is thus only slightly different from the corresponding expression for the centrosymmetric case. Therefore, the practical criteria discussed by Vand & Pepinsky will also hold here. Finally, it may be added that unlike the direct analytical relation between R and D available for the centrosymmetric case (see expressions (26) and (30) of Vand & Pepinsky, 1957) it has not been possible to obtain such an explicit relation for the non-centrosymmetric case.

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Polarization factor for X-ray monochromator crystals.

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The present authors recently carried out an absolute intensity measurement of X-ray reflexions from magnesium oxide powders, with Cu $K\alpha$ radiation monochromated by a curved lithium fluoride crystal using the 200 reflexion. The structure amplitudes derived therefrom are hereafter denoted as $F_{A,K}$. By an independent measurement with filtered Cu $K\alpha$ and Cr $K\alpha$ radiations, the relative values of structure amplitudes, F_R, were also obtained. Although $F_{A,K}$ and F_R are the quantities which are expected to be proportional to each other, a characteristic discrepancy from the proportionality was found as shown in Fig. 1, where $\log(F_{A,K}/F_R)$ is plotted against the scattering angle 2θ.

Such an anomaly seems to be ascribed to a misuse, in deriving $F_{A,K}$, of the polarization factor

$$p_K = \frac{1+\cos^2 2\theta_M \cos^2 2\theta}{1+\cos^2 2\theta_M} \qquad (1)$$

where θ_M is the Bragg angle at the monochromator.

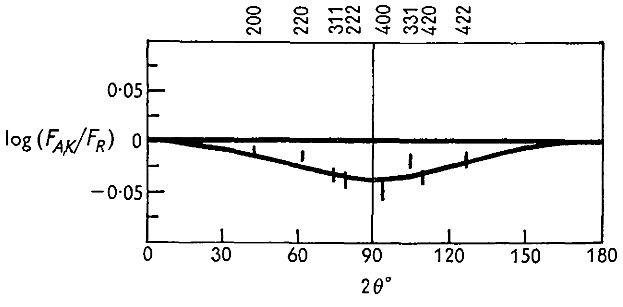

Fig. 1. $\log(F_{A,K}/F_R)$ against 2θ for magnesium oxide. $c=0{\cdot}6$.

The form (1) is valid when an ideally mosaic crystal is used as monochromator. If, however, the crystal is ideally perfect, we have to make use of the polarization factor

$$p_D = \frac{1+|\cos 2\theta_M|\cos^2 2\theta}{1+|\cos 2\theta_M|} \qquad (2)$$

(Kuriyama & Hosoya, 1963). In most cases the use of (1) may be approximately justifiable since monochromator

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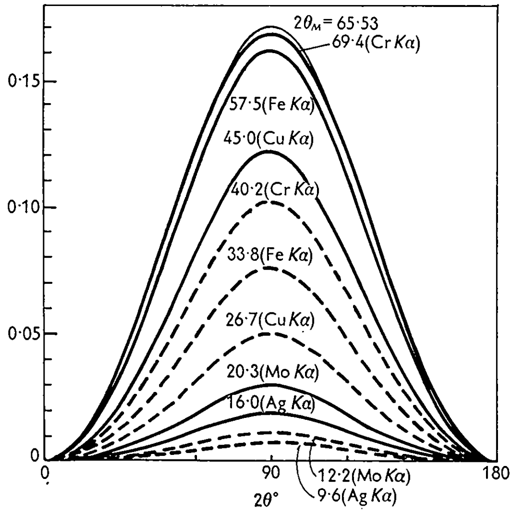

Fig. 2. $f(2\theta)$, with the values of $2\theta_M$ chosen so as to be appropriate to 200 of lithium fluoride (bold full line) and $10\bar{1}1$ of quartz (broken lines) for several kinds of ratiation.

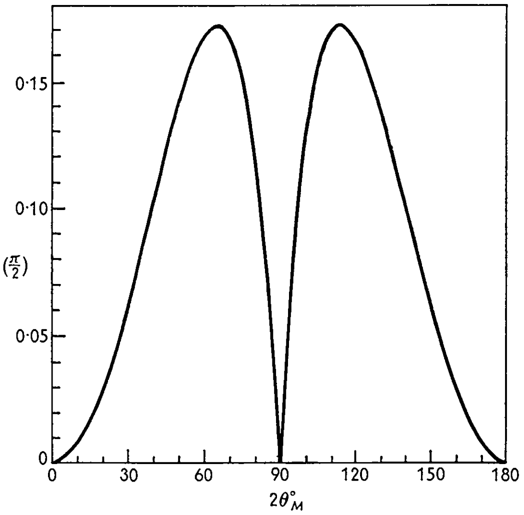

Fig. 3. $f(\pi/2)$ against $2\theta_M$.

crystals are usually with surfaces more or less ground in advance and are often bent crystals. However, the lack of exact knowledge about the perfectness of a monochromator may turn out to be a source of errors when a high accuracy is especially required for observed F values.

The correct values of the structure amplitudes F are to be derived with use of the correct form of the polarization factor p for the relevant monochromator crystal. $|F_{A,K}|$ is in general related to $|F|$ by

$$|F| = \sqrt{(p_K/p)}|F_{A,K}| \ .$$

Since $|F|$ should be proportional to $|F_R|$, we have

$$\log\left(|F_{A,K}|/|F_R|\right) = K + \tfrac{1}{2}\log\left(p/p_K\right) \tag{3}$$

where K is a constant. Although the exact form of p is usually unknown for a real crystal, which is generally an intermediate between ideally mosaic and ideally perfect, it will not be too unreasonable to assume phenomenologically that the crystal behaves, with respect to X-ray diffraction, as if it were composed of the perfect part and mosaic part with the fractions c and $1-c$, respectively. The form of p is then expressed as

$$p = cp_D + (1-c)p_K \ . \tag{4}$$

From (3) and (4) we obtain

$$\log\left(|F_{A,K}|/|F_R|\right) = K + \tfrac{1}{2}\log\left(c(p_D/p_K) + (1-c)\right) \ . \tag{5}$$

If c is small enough, equation (5) is approximated by

$$\log\left(|F_{A,K}|/|F_R|\right) = K - \tfrac{1}{2}cf(2\theta) \tag{6}$$

where $f(2\theta)$ is a function defined by

$$p_D/p_K = 1 - f(2\theta) \ . \tag{7}$$

The function $f(2\theta)$, which includes θ_M as parameter, is proved to be positive throughout, being symmetric about its maximum at $2\theta = \pi/2$. Fig. 2 shows the function $f(2\theta)$ for various values of $2\theta_M$, and Fig. 3, the peak value $f(\pi/2)$ as a function of $2\theta_M$. As seen in these figures, $f(\pi/2)$ attains its maximum value as large as about 0·1716 for $2\theta_M = 65{\cdot}53°$ and 114·47°. In particular the $f(\pi/2)$ value for 200 of lithium fluoride with Cu $K\alpha$ is about 0·12, as was also pointed out by Suzuki (1963) in his review article.

The solid curve in Fig. 1 corresponds to (6), with reasonably chosen values of K and c. The horizontal line is the level corresponding to K. Relation (6) may thus be used for estimating the correction to be applied to $|F_{A,K}|$. In the present example the magnitude of the correction amounts to about 3·5% at $2\theta = \pi/2$.

The above result shows that the extinction effect in monochromator crystals may sometimes have a non-negligible influence for accurate intensity measurements. The lithium fluoride monochromator used in the present study was of Johann type with a crystal which was bent at room temperature to the curvature $R = 26{\cdot}1$ cm and with a slightly ground surface. It is noticeable that the value of c obtained was still 0·6. This fact suggests that any monochromator crystal to be used for accurate intensity measurements should be examined in advance as to its polarization factor, although, as seen from Figs. 2 and 3, the ambiguity accompanying this factor may be substantially reduced by a suitable choice of θ_M.

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