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Polarization Ratios for Repeatedly Reflected X-ray Beams

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Abstract

The polarization ratio for a repeatedly reflected X-ray beam has been calculated, assuming the Darwin formulism, in the case where the diffracting planes of the crystals are parallel. It is shown that polarization ratios lie closer to unity than those obtained using the kinematic approximation. The integrated intensities and polarization ratios from a double-crystal spectrometer are discussed. The polarization ratio for a graphite monochromator has been measured experimentally and shown to be close to the value predicted by the Darwin theory and significantly different from the kinematic value.

Introduction

The degree of polarization which results from the scattering of an X-ray beam by a crystal depends on the polarization of the incident beam, the degree of perfection of the crystal and on the strength of interaction between the X-ray beam and the crystal, as well as the scattering angle. If the incident beam is unpolarized and the crystal is perfect, the polarization ratio, *i.e.* the ratio of the intensity scattered parallel to the diffraction plane to that scattered perpendicular to the diffraction plane, is $|\cos 2\theta|$, where θ is the Bragg angle. For an ideally mosaic crystal, to which the kinematic theory can be applied, the corresponding ratio will be $\cos^2 2\theta$. However, for a real mosaic crystal, where there is a strong interaction between the incident beam and the crystal, the kinematic theory will not apply and this will be particularly true if the diffracting crystal planes have a large structure factor and the crystal itself is large. Such a situation occurs when the crystal is being used as a monochromator or a focusing device and, in these cases, as has been pointed out by Jennings (1981), extinction theory applies.

Lawrence (1982) has shown that in the case of pyrolytic graphite, a commonly used monochromating material diffracting a large intensity from the (002) planes, the scattering can be described by the Darwin formulism. The reflectivity, R, in the symmetrical Bragg case, assuming no transmitted beam, is given by

$$R = \frac{\sigma + \mu/\gamma - [(\sigma + \mu/\gamma)^2 - \sigma^2]^{1/2}}{\sigma}.$$

σ is the reflectivity per unit length, γ is the direction cosine of the incident and diffracted beams and μ is the linear absorption coefficient. These are the symbols used by Weiss (1966). The reflectivity can be calculated separately for both polarizations, giving $R_{\parallel}$ and $R_{\perp}$ and thus the polarization ratio of the diffracted beam, $R_{\parallel}/R_{\perp}$, is found. The polarization ratio is thus a function of the mosaic spread of the crystal and the polarization ratios calculated in this manner are always greater than $\cos^2 2\theta$.

In this paper, the polarization factor of a repeatedly reflected X-ray beam is calculated and the measurement of the polarization ratio of a graphite crystal described.

Repeatedly reflected beam

The polarization factor for a repeatedly reflected beam has been studied by Vincent (1982). In the special case where the diffracting planes were parallel ($\rho = 0°$ geometry), it was shown that, if the crystals were

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ideally mosaic, the polarization factor, p_m, for a beam reflected m times, is

$$p_m = \frac{\prod_{i=1}^{m} \cos^2 2\theta_i + 1}{\prod_{i=1}^{m-1} \cos^2 2\theta_i + 1}.$$

Therefore, the polarization ratio, P_m, for the m-times-reflected beam will be

$$P_m = \prod_{i=1}^{m} \cos^2 2\theta_i.$$

If the crystals do not behave as ideally mosaic crystals and if the secondary extinction can be described by the Darwin formulism, the polarization ratio P'_m will be given by

$$P'_m = \frac{\prod_{i=1}^{m} R_{\parallel}(i)}{\prod_{i=1}^{m} R_{\perp}(i)}.$$

To determine P'_m, the mosaic spread and absorption factor of each crystal and the structure factor of each of the diffracting planes has to be known. A comparison between the values of the polarization ratios for the two theories can be made in the case of identical graphite crystals [the same as the single sample used by Lawrence (1982)] which have mosaic spreads of 0·26°. For Cu $K\alpha$ radiation ($\lambda = 1{\cdot}5418$ Å), $R_{\parallel} = 0{\cdot}426$, $R_{\perp} = 0{\cdot}465$ and $\cos^2 2\theta = 0{\cdot}799$ and, thus,

for $m = 2$	3	4,	
$P_m = 0.638$	0·510	0·408	
and $P'_m = 0{\cdot}839$	0·768	0·703.	

As can be seen, the kinematic approximation gives values of the polarization ratios which are too small and this will occur to a lesser or greater extent at all wavelengths and for all mosaic spreads. An increase in the mosaic spread would make the scattering more kinematic but would reduce the efficiency of the scattering.

Double-crystal spectrometer

Of particular importance is the case of a double-crystal spectrometer and the uncertainties which can arise from consideration of the polarization have been commented on by Evans, Leigh & Lewis (1977). The particular case of two identical parallel mosaic crystals will be considered, *i.e.* the (1, −1) mode, and it will be assumed that the incident beam is unpolarized. This situation corresponds to the $m = 2$ case discussed above.

The reflectivity, R_1, from the first crystal will be

$$R_1 = \frac{R_{\parallel} + R_{\perp}}{2}$$

and the two-reflection intensity, R_2, will be

$$R_2 = \frac{R_{\parallel}^2 + R_{\perp}^2}{R_{\parallel} + R_{\perp}}$$

and this can be expressed in terms of the polarization ratio as

$$R_2 = 2R_1 \frac{(1 + P^2)}{(1 + P)^2}.$$

A situation often arises where the first crystal remains stationary at its maximum reflection position and the second crystal is rotated through the Bragg reflection, of width $\Delta\theta$, and the total integrated intensity, ρ, measured.

Thus

$$\rho = \frac{R_{\parallel} \int R_{\parallel}(\Delta\theta)\mathrm{d}(\Delta\theta) + R_{\perp} \int R_{\perp}(\Delta\theta)\mathrm{d}(\Delta\theta)}{R_{\parallel} + R_{\perp}}.$$

The polarization of the final diffracted beam, P', will be given by

$$P' = \frac{R_{\parallel} \int R_{\parallel}(\Delta\theta)\mathrm{d}(\Delta\theta)}{R_{\perp} \int R_{\perp}(\Delta\theta)\mathrm{d}(\Delta\theta)}.$$

Fig. 1 shows the values of the calculated integrated intensities for graphite for a range of mosaic spreads at wavelengths up to 5·5 Å, assuming both crystals have

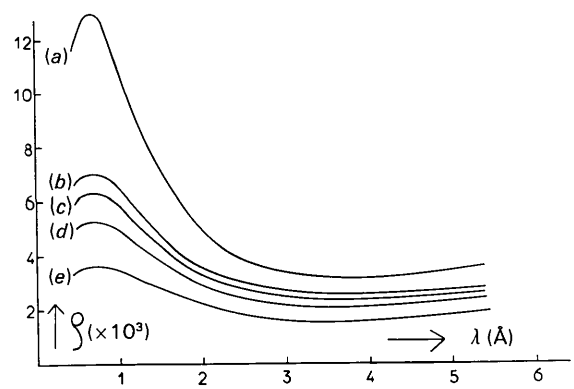

Fig. 1. The integrated intensities from a double-crystal spectrometer calculated (*a*) from the kinematic theory and (*b*)–(*e*) the Darwin formulism for crystals of mosaic spread (*b*) 1·0°, (*c*) 0·75°, (*d*) 0·5° and (*e*) 0·25°.

the same mosaic spread. The kinematic integrated intensities, ρ_k, calculated from

$$\rho_k = \frac{Q}{2\mu}\left(\frac{1+\cos^4 2\theta}{1+\cos^2 2\theta}\right)$$

are also shown.

The maximum, which occurs at about 0·7 Å, reflects the variation of the absorption coefficients of graphite with wavelength (Berry & Lawrence, 1979); the minimum occurs for a scattering angle of 45° where there is no parallel component reflected. The curves for the different mosaic spreads have their maximum and minimum values at approximately the same wavelengths and the curve associated with the greatest mosaic spread (1°) lies closest to the kinematic value. It should be noted, however, that, even for this large mosaic spread, the calculated integrated intensities were only, on average, half the kinematic value.

Fig. 2 shows the calculated polarization ratios for a range of scattering angles up to 45°, again assuming that both crystals have the same mosaic spread. Curves for mosaic spreads of 0·25 and 0·5° are shown and can be compared with the kinematic polarization ratios, $\cos^4 2\theta$. Curves for crystals of larger mosaic spreads, not shown here, would lie closer to this kinematic value. The curves for different mosaic spreads will not be exactly symmetrical about 45° since their exact shape depends on the absorption coefficient. The absorption coefficients used in the calculations were those of Berry & Lawrence (1979) (0·4 to 1·54 Å) and those of Hubbell (1977) (1·5 to 5·5 Å).

It should be emphasised that it has been assumed that the crystals were sufficiently thick that there was no transmitted beam. Otherwise, correction terms have to be applied to R and ρ_k.

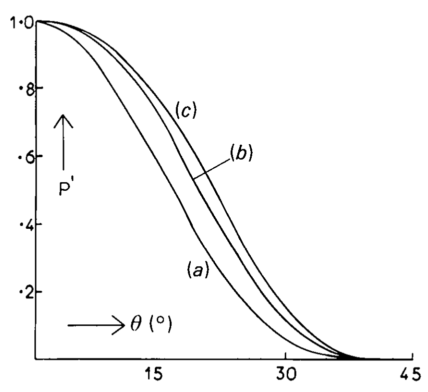

Fig. 2. The polarization ratio P' of a beam from a double-crystal spectrometer at scattering angle θ calculated from (*a*) the kinematic theory and (*b*), (*c*) the Darwin formulism with crystals of mosaic spread (*b*) 0·5° and (*c*) 0·25°.

Experimental

The polarization ratio was measured for the graphite crystal used by Lawrence (1982) using a simplification of the method used by Le Page, Gabe & Calvert (1979). The beam from an X-ray tube was diffracted by the crystal and then re-scattered by a uniform piece of transparent plastic, the intensities from the plastic in directions parallel to and perpendicular to the diffracting planes of the crystal being measured separately. The ratio of these intensities gives the polarization ratio and, for Cu $K\alpha$ radiation, the experiments were performed three times, giving values of 0·871, 0·883 and 0·886. For each experiment, at least 100 000 counts were accumulated for each intensity and the polarization ratio can be taken to be 0·88 (1). The values obtained from the Darwin theory were 0·916, assuming purely reflection processes, and 0·892, assuming integration processes. The better agreement between the integrated polarization ratio and experimental result is not surprising in view of the highly divergent main beam which was used.

An attempt to repeat the experiment for Mo $K\alpha$ radiation was not successful; a polarization ratio significantly different from unity could not be measured. This, however, emphasises that the polarization ratio is not $\cos^2 2\theta$.

Conclusion

The assumption that the polarization ratio of a singly diffracted beam is $\cos^2 2\theta$ is incorrect and, using the Darwin formulism, the polarization ratio of a repeatedly reflected beam can be deduced. An experimentally determined polarization ratio gives good agreement with the theory.

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