

remarkable correspondence between the two sets of quantities indicates that the crystal is essentially one individual, without significant twinning of the kind described above. Indeed, assuming a fraction, q , of incoherent inverse domains to be present, one calculates a set of corrected $|F_c|^2$ values: $|F_c(+,\text{corr.})|^2 = |F_c(+)|^2 - q[|F_c(+)|^2 - |F_c(-)|^2]$, and $|F_c(-,\text{corr.})|^2 = |F_c(-)|^2 + q[|F_c(+)|^2 - |F_c(-)|^2]$; a least-squares calculation of q , then, from the data in Table 3 yields $q = 0.15 \pm 0.07$. As seen from the table, however, R improves very little: from 0.939 to 0.927. A Hamilton test of the ratio $\mathcal{R}_o = 0.939/0.927 = 1.013$ leads to rejection, with more than 50% probability, of the hypothesis that this is a real observation of 15% incoherent inverse domains; for $\mathcal{R}_o = 1.013$ is much less than $\mathcal{R}_{1,10,0.50} = 1.024$. Furthermore, the quantity that could be designated

$$R_{\Delta} = \frac{100 \sum ||F_o(+)| - |F_o(-)|| - ||F_c(+)| - |F_c(-)||}{\sum ||F_o(+)| - |F_o(-)||}$$

actually increases from 22 to 27% when q is changed from 0 to 0.15.

It is obvious, of course, that occurrence of this type of twinning should be of no consequence whatsoever for the precise refinement of γ -brass or similar structures.

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A Method of Eliminating the Polarization Ratio of a Crystal Monochromator as an Interactive Constant in the Polarization Factor

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Disposition of a monochromator crystal relative to the specimen crystal on a diffractometer, such that the respective diffraction planes are at 45° , makes knowledge of the actual value of the polarization ratio for the monochromator crystal unnecessary for the conversion of measured intensities to structure-factor values for the specimen crystal. This arrangement, therefore, avoids the uncertainty often associated with poor knowledge of the polarization ratio of monochromator crystals, and so can contribute to improved accuracy of measured structure factors.

Introduction

In recent years, the combination of a crystal monochromator with a diffractometer has been used with the aim of improving the accuracy of structure factor values derived from measured intensities of the crystal specimen. For the attainment of this aim, it has been assumed that an accurate value of the polarization ratio appropriate to the monochromator crystal was necessary. Establishment of such values has not proved straightforward (International Union of Crystallography, 1978). The reason is that, for real crystals, the required parameter is not a simple function of $\cos 2\theta$, such as $\cos^2 2\theta$, where $r = 1$ or 2 (which would apply if dynamical or kinematical theory, respectively, were exactly applicable), but is the ratio, I_π/I_σ , of the diffracted power of the π component to that of the σ component for the set position of the monochromator.* Because of the inevitable presence of extinction, this intensity ratio is dependent on factors other than $\cos 2\theta$, such as F and λ , the structure factor value and the radiation wavelength respectively. Indeed the ratio can be of considerable value as an indicator of the comparative extinction levels of the π and σ components of the particular reflexion used as monochromator (Chandrasekhar, Ramaseshan & Singh, 1969; Olekhovich, Rubtsov & Shmidt, 1975). Hence it is not surprising that the search for a single reference value of the polarization ratio, applicable in general for a given material at a particular wavelength, has proved abortive and may, indeed, be illusory.

There is, however, a relatively simple variant of the disposition of the monochromator crystal relative to that of the specimen crystal such that knowledge of the actual numerical value of the polarization ratio for the monochromator crystal becomes unnecessary.

Net polarization factor as a function of the mutual disposition of two crystals

Consider an unpolarized X-ray source and two crystals, X_1 and X_2 , in series, Fig. 1(a). Let the polarization ratios for the two crystals be K_1 and K_2 , where $K_n = I_{\pi n}/I_{\sigma n}$. For the general case where the plane of diffraction of the second crystal is at an angle ϕ to the plane of diffraction of the first, Fig. 1 (cf. Mathieson, 1968), the polarization factor, $P_{1,2}(\phi)$, of the overall system, $X_1 + X_2$, in relation to the source is given by

$$P_{1,2}(\phi) = \frac{(\cos^2 \phi + K_1 \sin^2 \phi) + (\sin^2 \phi + K_1 \cos^2 \phi)K_2}{1 + 1}$$

* Only in the case of vanishingly small F , and indeed only exactly for $F = 0$ (Mathieson, 1977), does the polarization ratio, I_π/I_σ , become equal to the ratio of the polarization components, $(\cos^2 2\theta)/1$. Here, we are dealing with strong reflexions and so are far from that limit.

For the standard configurations, (a) where the planes of diffraction are coincident, $\phi = 0^\circ$, and (b) where they are at right angles, $\phi = 90^\circ$ (Furnas & Beard, 1965), this simplifies to

$$P_{1,2}(0^\circ) = \frac{1 + K_1 K_2}{2}$$

and

$$P_{1,2}(90^\circ) = \frac{K_1 + K_2}{2}.$$

These are forms which are well-known and for the application of which knowledge of the polarization ratio of the monochromator crystal, whether K_1 or K_2 , is necessary, since it is an interactive constant in both cases. For $\phi = 45^\circ$, the expression takes the form,

$$P_{1,2}(45^\circ) = \frac{(1 + K_1)(1 + K_2)}{4},$$

which has an interesting consequence. If one of the crystals is acting as the monochromator, its polarization ratio, K_m , is constant while that for the specimen crystal varies as different reflexions are selected and is, in a broad sense, functionally dependent on 2θ , i.e. $K_s(2\theta)$, (as well as on the other factors which determine diffracted intensity, see *Introduction*). Then

$$\begin{aligned} P_{m,s}(45^\circ) = P_{s,m}(45^\circ) &= \frac{(1 + K_m)[1 + K_s(2\theta)]}{4} \\ &= C[1 + K_s(2\theta)], \end{aligned}$$

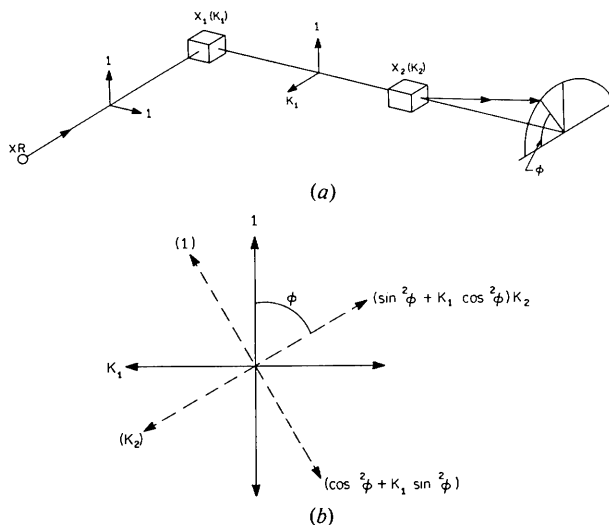


Fig. 1. (a) A diagram showing X-rays from an unpolarized source, XR, being diffracted first from crystal X_1 , and then from crystal X_2 . The reflexion plane for X_2 is visualized as variable and adjustable to any given value, ϕ , see Fig. 2(b) in Mathieson (1968). The polarization components for the incident and diffracted beams of X_1 are indicated while those for X_2 are given in: (b) an illustration of the relation between the polarization components incident on X_2 , 1 and K_1 , and those of the beam diffracted by X_2 , $(\cos^2 \phi + K_1 \sin^2 \phi)$ and $(\sin^2 \phi + K_1 \cos^2 \phi)K_2$, for the case of the reflexion planes being tilted at a general angle ϕ relative to one another.

and K_m is absorbed as a scale factor. With this configuration, knowledge of the numerical magnitude of K_m is no longer required.

It will be noted that the various forms of the expression are symmetrical in respect of K_1 and K_2 so that, as far as the polarization ratio is concerned, the question of whether it is an *ante*-monochromator or a *post*-monochromator arrangement (Mathieson, 1968) is not, in that respect, critical.

In an operational sense, the relative sequence of the monochromator and specimen crystals may lead to differences. Where only relative values of intensities are sought, there is virtually no distinction. If, however, absolute intensities are the aim, there is an advantage in the case of the *ante*-monochromator (case I, Mathieson, 1968). With this configuration, one can measure the intensity of the beam incident on the specimen crystal, since that is monochromated, and the polarization factor for the specimen crystal alone is

$$P_s = \frac{(1 + K_m)[1 + K_s(2\theta)]}{1 + K_m} \\ = 1 + K_s(2\theta).$$

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Interaction Energies at Twin Boundaries and Effects of the Dihedral Reentrant and Salient Angles on the Growth Morphology of Twinned Crystals

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Twin-boundary energies are calculated with the Lennard-Jones 6–12 potential function for the (110) and (310)-twin laws of orthorhombic even *n*-alkane crystals. In agreement with experiment, the calculations show that the higher the interaction energy along the twin boundary, the higher the probability of observing the corresponding twin. According to the values of the reentrant angles, the adsorption sites near the twin boundary may act as permanent growth sites (kinks) where growth takes place spontaneously and leads to a crystal elongated in the direction of the twin boundary.

1. Introduction

A peculiar aspect of the growth of twinned crystals showing dihedral reentrant and salient angles is the change of the normal growth kinetics of the faces which

In conclusion, it is interesting to note that although Kirkpatrick (1927) made an observation, in a similar vein, concerning how to deal with the possibility of the X-rays from an X-ray tube being polarized, its significance for the use of monochromator crystals has not apparently been commented on over the last half-century.

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form these angles. Generally, the occurrence of a reentrant angle is followed by an increase of the growth kinetics; this phenomenon was observed on different crystalline species (Frank, 1949; Stranski, 1949). To our knowledge, no kinetic measurements have been