

this has been previously observed in some copper- and silver-base alloys (Davies & Cahn, 1962; Adler & Wagner, 1962; Goswami *et al.*, 1966; Sen Gupta, 1967). However, it may be mentioned that the fault probability  $\alpha$  has been obtained from neighbouring pairs of reflexions and the average value of  $\alpha$  has been considered in the present case, whereas in the earlier measurements of  $\alpha$  for Cu-In, Cu-Sn alloys (Goswami *et al.*, 1966) only the first pair of reflexions were considered.

The twin fault probability  $\beta$  also increases with increasing solute content (Fig. 1) and it is observed that apart from the limitations which exist in the determination of  $\beta$  (Sen Gupta & Quader, 1966), the trend of variation is similar in all cases attaining saturation at higher solute content, and for a fixed amount of solute present  $\beta$  also increases in the order Cu-In, Cu-Sn, Cu-Sb.

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## Crystal Setting by Rotation Photographs

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Applications are described of a simplification and generalization of Roof's method of setting single crystals by rotation photographs. The method is particularly recommended for setting irregular fragments of known unit cell to a specified axis.

Roof (1955) has described a method of setting triclinic crystals to a zone axis by taking three trial rotation photographs, making shifts  $\delta\alpha^\circ$ ,  $\delta\beta^\circ$  on the two goniometer arcs in turn between exposures. If  $\delta\alpha$  and  $\delta\beta$  are reasonably small, equivalent reflexions can be recognized on the three photographs. By selecting two prominent low-angle reflexions near the equator, measuring their departures from the equator as  $\tan N = \zeta/\xi$  in each of the six cases, and using the nomogram given by Roof, one derives arc corrections which bring the two reflexions onto the equator exactly, and thus to coincide with their equivalent reflexions previously below the equator. The crystal is then set to a zone axis, and if the two reflexions were properly selected initially, the axis will probably be a prominent one.

Roof's method has now been superseded by that of Brooker & Nuffield (1966) who use a similar triplet of rotation photographs, but taken in a flat-film camera; they show how one may transfer data for any number of recorded reflexions to a stereogram of the crystal in its random setting, from which one may deduce symmetry if any, and more reliable positions for the main zone axes. Their method is relatively labori-

ous, however, and I have found the following simplification and generalization of Roof's method useful on several occasions.

#### Theoretical

The method depends on the essentially empirical observation that if the separation between a pair of equivalent reflexions is measured with a ruler, then to a good approximation it plots as a plane on a square mesh of  $\alpha$  and  $\beta$ , the goniometer arc readings.

Consider the crystal in terms of spherical polar coordinates on the required zone axis as origin. The planes giving rise to the (coincident) spots on the rotation photograph are then at  $(\varphi, \varrho)$ ,  $(-\varphi, \varrho)$  respectively. If the crystal is rotated to some other rotation axis, having coordinates  $(\varphi', \varrho')$  on this coordinate system, the planes now have  $\varrho$ -values,  $\varrho_1, \varrho_2$ , given by:

$$\cos \varrho_1 = \cos \varrho \cos \varrho' + \sin \varrho \sin \varrho' \cos (\varphi' + \varphi)$$

$$\cos \varrho_2 = \cos \varrho \cos \varrho' + \sin \varrho \sin \varrho' \cos (\varphi' - \varphi).$$

Subtracting:

$$2 \sin \frac{1}{2}(\varrho_1 + \varrho_2) \sin \frac{1}{2}(\varrho_1 - \varrho_2) = 2 \sin \varrho \sin \varrho' \sin \varphi \sin \varphi'.$$

Rotations of the crystal in the direction  $\varphi' = 0^\circ$  or  $180^\circ$

leave  $\varrho_1 = \varrho_2$  and the spots are still coincident, whence this direction is a contour of zero separation. For rotations within the range of the arcs,  $\sin \varrho' \sin \varphi' \approx \varrho' \sin \varphi'$  measures the perpendicular distance of the axis from this line on a Wulff net on which the arc coordinates are plotted. Since the centre of a Wulff net is nearly a square mesh, and since  $\varphi$  and  $\varrho$  are constants,  $2 \sin \frac{1}{2}(\varrho_1 - \varrho_2)$  can be plotted approximately as a plane on a square mesh of  $\alpha$  and  $\beta$ , provided  $\sin \varrho / \sin \frac{1}{2}(\varrho_1 + \varrho_2)$  is reasonably constant. In so far as a Bernal chart is a square mesh in  $\xi$  and  $\zeta$ , the quantity measured with a ruler is proportional to  $2 \sin \frac{1}{2}(\varrho_1 - \varrho_2)$ . For  $\varrho = 90^\circ$  (equatorial reflexions)  $\sin \varrho / \sin \frac{1}{2}(\varrho_1 + \varrho_2)$  is exactly constant; the present method is almost exact and supersedes Roof's method. As  $\varrho$  decreases,  $\sin \varrho / \sin \frac{1}{2}(\varrho_1 + \varrho_2)$  is less constant within the range of the arcs, but no difficulty has been experienced for reflexions at  $\varrho$ -values of  $54^\circ$  (see ferritungstite below). Inspection of the charts mentioned above suggests that the approximations are mutually compensating. In particular as  $\frac{1}{2}(\varrho_1 + \varrho_2)$  decreases, the quantity measured (along the constant  $\theta$  contour) exceeds ever more the function  $\sin \frac{1}{2}(\varrho_1 - \varrho_2)$  thus compensating for the increase in the  $\sin \varrho / \sin \frac{1}{2}(\varrho_1 + \varrho_2)$  term. A more exact analysis is too cumbersome to be worth while.

### Practical

Despite the crudity of the approximations, I have found they work well in practice for reasonably low-angle reflexions (say  $\xi < 1$ ,  $\zeta < 0.5$ , reflexions not too near the trace of the rotation axis), and they form a practical method of crystal setting. For example one might read for a particular pair of reflexions:

<i>P.</i>	<i>T</i> $0^\circ$	<i>B</i> $0^\circ$	Separation = 3.0 mm
<i>Q.</i>	<i>T</i> $0^\circ$	<i>B</i> $5^\circ\text{R}$	Separation = 2.2 mm
<i>R.</i>	<i>T</i> $5^\circ\text{R}$	<i>B</i> $5^\circ\text{R}$	Separation = 2.8 mm

Fig. 1 represents arc coordinates on a square mesh. On the auxiliary graph one plots the separations at *P* and *Q* against bottom arc reading, and from the straight line thus obtained one reads *X*, the point at which the separation equals that at *R*, and *Y*, the point of zero separation. *X* and *Y* are transferred as *AY* parallel to *RX*. The zero contour is then estimated as *AY* parallel to *RX*.

For the three trial photographs it is advisable to keep the shifts  $\delta\alpha$ ,  $\delta\beta$ , reasonably small, say  $5^\circ$ . The spot separation is strictly a vector which may change sense undetectably when the spots cross over between photographs. Owing to the approximations involved, great accuracy of measurement is wasted, and measurements made to 0.1 mm with a scale on the wet film by naked eye suffice. It is advisable to plot the auxiliary graph parallel to the arc having greatest effect on the separation.

From a second pair of reflexions one similarly derives a second zero contour, say *AM* in Fig. 1. *A* then gives the approximate settings for the corresponding zone axis. *A* is unlikely to be exact but would suffice as a

basis for refinement by double oscillation photographs, provided the reflexions have not crossed over (I have yet to meet this situation).<sup>\*</sup> Alternatively one may take a fourth trial rotation photograph with the crystal deliberately misset by a few degrees from *A*,<sup>†</sup> in the field defined by the zero contours and the origin. The small separations now measured can be projected back onto the lines of the auxiliary graphs, using the present zero contours, transferred to the auxiliary graphs, and there used to find revised positions of *Y* (and *M*) in Fig. 1, and hence a revised position for *A*. This should now be sufficiently accurate to give a reasonable rotation photograph.

I have found this method works efficiently in bringing selected pairs of equivalent reflexions into coincidence. For example it offers a convenient simplification of Roof's method, for triclinic crystals. The mathematical theory of Roof's method becomes impossibly cumbersome for off-equatorial coincidences. These arise when a crystal of higher symmetry is set to a symmetry axis, when its rotation photograph consists of pairs (or more) of coincident reflexions on all layer lines. The present method is equally applicable to off-equatorial coincidences.

<sup>\*</sup> The referee suggests that it is always preferable to consider more than two reflexions in Fig. 1. This would also act as a useful precaution against cross-over, when the zero contours would fail to meet near a point. It would also give a better approximation to *A* when working at low  $\varrho$ -values.

<sup>†</sup> The amount of missetting will vary with  $\varrho$ -value. Near the equator it can be quite small; at very low  $\varrho$ -values *A* should be approached more cautiously.

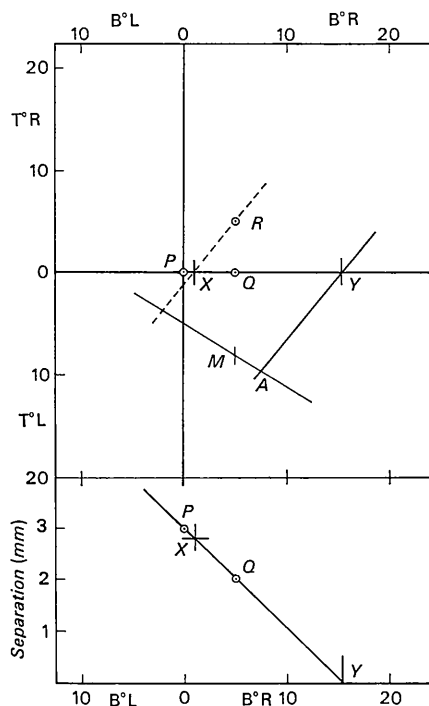


Fig. 1. Working diagram for crystal setting by rotation photographs. For explanation see text.

In the use of this method as a setting method the main difficulty arises in selecting the reflexions to be brought into coincidence. This does not arise with irregular fragments of known unit cell (e.g. ground spheres), and the method may then prove superior to others. For example a colleague setting an irregular crystal of (?) face-centred cubic ferritungstite to [100] repeatedly converged on [111] by trial oscillation photographs. We had no difficulty in bringing two pairs of 111 reflexions into off-equatorial coincidence by this method, thus setting to the required axis. In some similar cases it may well happen that the predicted position of  $A$  in Fig. 1 lies outside the range of the arcs. The prediction will then be rather inaccurate owing to departures from the approximations above, but should suffice to indicate how the crystal should be remounted for a further triplet of trial rotation photographs. The indication of azimuth is likely to be more accurate than that of the inclination. It may be preferable to locate another known axis, accessible to the arcs, and derive the inclination from this.

Most workers use trial oscillation (or Laue) photographs for normal crystal setting, when using an irregular fragment. It is well known that recognizing badly missed layer lines is a knack, to be acquired by practice. The writer derived this method for general use before acquiring this knack, to study serendibite (Prior & Coomáraswámy, 1903; cf. Pertzev & Nikitina, 1959) available as type material in the form of rough irregular fragments thought to be triclinic. The

above method was triumphantly successful at first attempt, setting a crystal on to an axis displaying equatorial symmetry on even-order, but not on odd-order layer lines, by using off-equatorial coincidences. The axis proved to be [122] of the reduced all-acute triclinic cell.

Subsequent use suggests that this success was partly accidental. The difficulty lies in properly selecting the reflexions to be brought into coincidence. Choice of off-equatorial coincidences if possible will favour setting to a symmetry axis if any exists. It seems likely that extending Fig. 1 to consider more than two reflexions, thus obtaining a consensus, offers best chance of success. The method used in these circumstances is simple and offers as much chance of quick success as trial oscillation photographs, but for general setting of irregular fragments, the method of Brooker & Nuffield, while more elaborate, is more certain. However, where the unit cell of the irregular fragment is known, the present method offers many advantages over other recommended photographic methods.

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## The Decomposition of an Anisotropic Elastic Tensor

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The classical theory of invariants asserts that there exists a finite integrity basis whose elements are polynomials of strain components and are invariant under the group of transformation defining each symmetry class of a crystal. By constructing a strain energy function made up of the elements of an integrity basis for a certain symmetry class, we derive a tensor basis which spans the space of elastic constants for crystals of this symmetry class. Introducing systematically new elements of the integrity basis into the construction of the strain energy function, we construct five hierarchies of orthonormal tensor bases which span the space of the second-order elastic constants of all crystal systems. Any elastic tensor of rank four possessing certain crystallographic symmetry may be decomposed into a sum of tensors of increasing symmetry. From this representation of an anisotropic elastic tensor, the tensor of any given symmetry, not only the isotropic one, nearest the given tensor can be read off immediately. Bases which span the space of elastic constants of orders higher than the second may be computed in a similar manner. Such computations can be carried out by a computer. A FORMAC program of 7090/94 IBSYS has been written to obtain the elastic constants of the second and the third order for each class of a crystal.

### 1. Introduction

In an investigation of the physical properties of an anisotropic body, one sometimes begins with the cor-

responding properties of an isotropic body having the same geometry and proximal constitutive physical relations, and for which some knowledge may be obtainable with relative ease. It may then be possible to