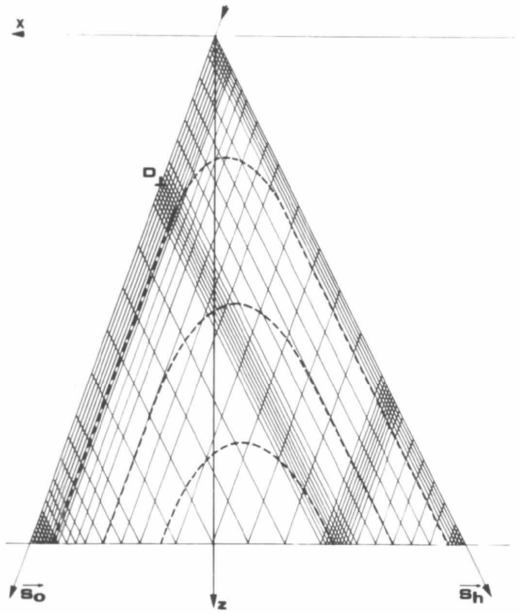

Fig. 1. Principles of the integration network.

When the defect possesses a direct image, its shape is roughly calculated according to the kinematical theory (Authier, 1967) and the length of the integration step is decreased in the corresponding area (Fig. 1).

The Takagi–Taupin equations are then integrated. The program automatically switches from an integration network taking into account the direct image to another one without it, when it is needed. This automatic adaptation of the program to the diffraction conditions permits the simulation of the section topograph of a dislocation with high accuracy. We have been able, for example, to determine the direction of the Burgers vector of a dislocation through the features of its direct image (Fig. 2).

Thus it is now possible to simulate section topographs with good accuracy in all parts of the image. More details about this new routine *DEFV* will be given in a further paper.

Topograph shown in Fig. 2 is from Dr M. Lefeld-Sosnowska (University of Warsaw). Its contrast will be discussed in a work currently in progress in collaboration with A. Authier.

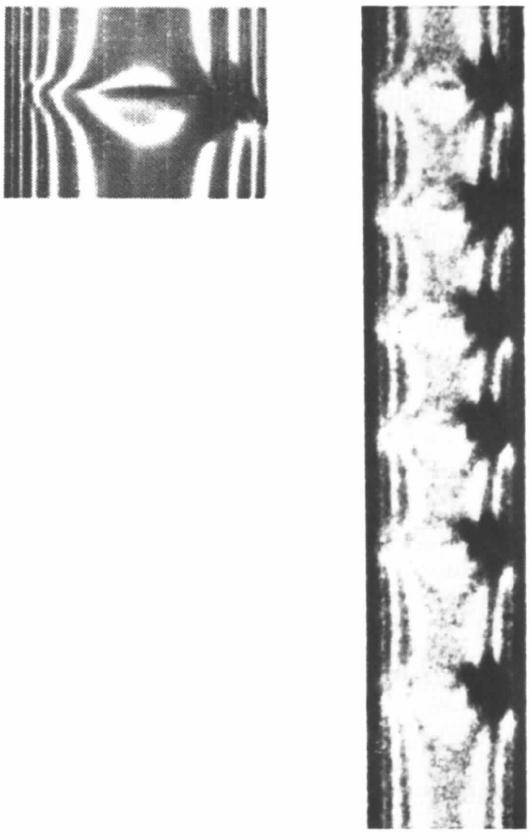

Fig. 2. Section topograph of a silicon wafer, Mo $K\alpha$, $33\bar{3}$.

References

AUTHIER, A. (1967). *Adv. X-ray Anal.* **10**, 9–31.
AUTHIER, A., MALGRANGE, C. & TOURNARIE, M. (1968). *Acta Cryst.* A**24**, 126–136.
EPELBOIN, Y. (1977). *Acta Cryst.* A**33**, 758–767.
PETRASHEN, P. V. (1976). *Fiz. Tverd. Tela* (*Leningrad*), **18**, 3729–3731.
TAUPIN, D. (1964). *Bull. Soc. Fr. Mineral. Cristallogr.* **87**, 469–511.

Acta Cryst. (1981). A**37**, 133–135

A general rule for origin specification in any space group.

By SVEN HOVMÖLLER, *Department of Structural Chemistry, Arrhenius Laboratory, University of Stockholm, S*-106 91 *Stockholm, Sweden*

(*Received* 2 *June* 1980; *accepted* 1 *September* 1980)

Abstract

A general and simple rule for the derivation of which reflections should be used for fixing the origin in any of the 230 space groups is given.

The number of reflections needed to specify the origin is identical to the number of elements in the seminvariant vector of that space group. For example, in $P2_12_12_1$, the seminvariant vector is (hkl) modulo (2 2 2). Thus three reflections are needed to specify the origin. In $P4$ the seminvariant vector is $(h + k, l)$ modulo (2,0) and two

0567-7394/81/010133-03$01.00

reflections are needed to specify the origin. Seminvariants are tabulated by Hauptman & Karle (1956, 1959), Giacovazzo (1974), Karle (1974, pp. 339–358), Lessinger (1975) and Hovmöller (1978). The kinds of reflections that will specify (or fix) the origin can be derived from the seminvariant vector and modulus (Hauptman & Karle, 1956). The following rule holds:

A set of reflections specify the origin if and only if they are linearly independent and primitive relative to the seminvariant modulus (ω_s).

This rule may be turned into a simple method to determine whether a given set of reflections will specify the origin or not.

1. Reduce all indices of the reflections modulo the elements of the seminvariant vector.
2. Make an $n \times n$ matrix of the n reduced reflections used for origin specification.
3. If there are one or two polar axes the rows (but not the columns) of the matrix may be subtracted from each other in order to reduce the indices to 0 or 1 if possible. All indices may again be reduced modulo the seminvariant vector between each such subtraction.
4. If it is possible to reduce the matrix down to where its determinant is +1 or −1, then the origin is fixed, otherwise not.

The moduli function is such that n (modulo m) means that m is subtracted from n until a number j, $0 \le j < m$, is reached. Thus 2 (modulo 2) = 0, 7 (modulo 0) = 7 and 35 (modulo 3) = 2.

The method presented here is a generalization of all the different rules for origin specification in specific space groups, such as those tabulated by Karle (1974, pp. 345–349).

Example $P2_12_12_1$

Does the set of reflections (5,14,7), (3,3,3) and (5,6,8) fix the origin?

1. Reduce all indices modulo (2,2,2): (1,0,1), (1,1,1) and (1,0,0).
2. Make an $n \times n$ matrix of the vectors above:

$$\begin{pmatrix} 1 & 0 & 1 \\ 1 & 1 & 1 \\ 1 & 0 & 0 \end{pmatrix}.$$

3. There are no polar axes (no moduli are = 0) so we continue with 4.
4. The determinant is calculated to be $= 0 + 0 + 0 - 0 - 1 - 0 = -1$ and the origin is fixed.

Example Pm

Is the origin fixed by the reflections (5,1,7), (7,3,2) and (0,9,1)?

1. Reduce all indices modulo (0,2,0): (5,1,7), (7,1,2) and (0,1,1).
2. The $n \times n$ matrix will become:

$$\begin{pmatrix} 5 & 1 & 7 \\ 7 & 1 & 2 \\ 0 & 1 & 1 \end{pmatrix}.$$

3. There are two polar axes (x and z) and we may reduce the matrix:

$$\begin{pmatrix} 5 & 1 & 7 \\ 7 & 1 & 2 \\ 0 & 1 & 1 \end{pmatrix} \rightarrow \begin{pmatrix} 5 & 1 & 7 \\ 2 & 0 & -5 \\ 0 & 1 & 1 \end{pmatrix} \rightarrow \begin{pmatrix} 1 & 1 & 17 \\ 2 & 0 & -5 \\ 0 & 1 & 1 \end{pmatrix} \rightarrow \begin{pmatrix} 1 & -16 & 0 \\ 2 & 0 & -5 \\ 0 & 1 & 1 \end{pmatrix} \rightarrow \begin{pmatrix} 1 & 0 & 0 \\ 2 & 0 & -5 \\ 0 & 1 & 1 \end{pmatrix} \rightarrow \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & -5 \\ 0 & 1 & 1 \end{pmatrix} \rightarrow \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 1 & 1 \end{pmatrix}.$$

4. The determinant is equal to −1 and the origin is fixed.

*Example P*4

The seminvariant vector of $P4$ is $(h + k, l)$ modulo (2,0). Since there are only two elements of the seminvariant vector the origin may be specified by only two reflections.

Try (5 1 7) and (7 1 2).

1. The h and k indices should be added as is seen from $(h + k, l)$. We get (5 + 1, 7) and (7 + 1, 2) or (6,7) and (8,2). These are reduced modulo (2,0) to give (0,7) and (0,2).
2. The 2 × 2 matrix becomes

$$\begin{pmatrix} 0 & 7 \\ 0 & 2 \end{pmatrix}.$$

3. Already, before reduction of the matrix, we see that the determinant will be = 0, and the origin is not fixed.

Try another set of reflections: (5,14,7) and (3,3,3).

1. (5 + 14, 7) and (3 + 3, 3) are (19,7) and (6,3). When reduced modulo (2,0) we get (1,7) and (0,3).
2. The 2 × 2 matrix becomes

$$\begin{pmatrix} 1 & 7 \\ 0 & 3 \end{pmatrix}.$$

3. The matrix may be reduced according to:

$$\begin{pmatrix} 1 & 7 \\ 0 & 3 \end{pmatrix} \rightarrow \begin{pmatrix} 1 & 1 \\ 0 & 3 \end{pmatrix} \rightarrow \begin{pmatrix} 1 & 1 \\ -3 & 0 \end{pmatrix} \rightarrow \begin{pmatrix} 1 & 1 \\ 1 & 0 \end{pmatrix}.$$

4. The determinant is equal to −1 and the origin is fixed.

*Example P*6

The seminvariant vector of $P6$ is $(2h + 4k + 3l)$ modulo (6) (Hovmöller, 1978). Only one reflection is needed to specify the origin.

Try (5 1 7).

1. $(2 \times 5 + 4 \times 1 + 3 \times 7) \quad 35 = -1$ modulo 6, and the origin may be fixed by this reflection.

References

GIACOVAZZO, C. A. (1974). *Acta Cryst.* A**30**, 390–395.

HAUPTMAN, H. & KARLE, J. (1956). *Acta Cryst.* **9**, 45–55.

HAUPTMAN, H. & KARLE, J. (1959). *Acta Cryst.* **12**, 93–97.

HOVMÖLLER, S. (1978). *Acta Cryst.* A**34**, 826–827.

KARLE, J. (1974). In *International Tables for X-ray Crystallography*, Vol. IV. Birmingham: Kynoch Press.

LESSINGER, L. (1975). *Acta Cryst.* A**31**, 521.

Acta Cryst. (1981). A**37**, 135–137

Molecular orientation distribution derived from an arbitrary reflection.

By R. LOVELL and G. R. MITCHELL, *Department of Metallurgy and Materials Science, University of Cambridge, Pembroke Street, Cambridge CB2 3QZ, England*

(*Received* 24 *June* 1980; *accepted* 5 *August* 1980)

Abstract

A straightforward method using Legendre series enables the orientation distribution in a specimen with uniaxial symmetry to be derived from the azimuthal profile of a single arbitrary reflection. Moreover, the moments of the distribution $\langle P_{2n}(\cos\alpha)\rangle$ can be obtained directly from the azimuthal profile without needing to calculate the complete distribution.

Pole figures derived from X-ray diffraction measurements are the standard method of quantifying orientation in crystalline materials. Similarly, the azimuthal profiles of the diffuse arcs found for liquid crystals (Leadbetter & Wrighton, 1979) and non-crystalline polymers (Wilchinsky, 1968) have been used to give a measure of orientation.

In polymers and liquid crystals, it is usually the orientation distribution for the molecular axes which is required, but this is only obtained directly from a pole figure if there is a strong reflection from planes perpendicular to the molecular axes. However, Wilchinsky (1963) has shown that, provided the molecules are random about their axes, a single arbitrary reflection can give the value of $\langle\cos^2\alpha\rangle$, where α is the angle between the molecular axis and the specimen axis.

In this communication we show that, for a specimen with uniaxial symmetry, the higher moments of the orientation distribution can also be obtained from the azimuthal profile of an arbitrary reflection. Hence the full orientation distribution can be calculated without recourse to solving integral equations or inverting matrices.

The scattering from a distribution of independent molecules is given by a convolution of the orientation distribution of molecular axes with the scattering for a single molecule (Ruland & Tompa, 1968). If both the orientation distribution $D(\alpha)$ and the molecular scattering $I^m(\alpha)$ have cylindrical symmetry, then the resultant scattering $I(\alpha)$ also has cylindrical symmetry (Deas, 1952) and all three functions can be expanded in series of even-order Legendre polynomials (P_{2n}), *e.g.*

$$I(\alpha) = \sum_{n=0}^{\infty} I_{2n} P_{2n}(\cos\alpha),$$

where

$$I_{2n} = (4n + 1) \int_0^{\pi/2} I(\alpha) P_{2n}(\cos\alpha) \sin\alpha \, d\alpha.$$

Similar formulae apply to $D(\alpha)$ and $I^m(\alpha)$.

It has been shown (Deas, 1952) that the coefficients of the three series are related by

$$I_{2n} = \frac{2\pi}{4n + 1} D_{2n} I^m_{2n},$$

which implies that

$$\langle P_{2n}\rangle_I = \langle P_{2n}\rangle_D \langle P_{2n}\rangle_{I^m},$$

where

$$\langle P_{2n}\rangle_I = \frac{\int_0^{\pi/2} I(\alpha) P_{2n}(\cos\alpha) \sin\alpha \, d\alpha}{\int_0^{\pi/2} I(\alpha) \sin\alpha \, d\alpha}. \qquad (1)$$

Hence, if $I(\alpha)$ and $I^m(\alpha)$ are known, we can derive the orientation parameters of the distribution:

$$\langle P_{2n}\rangle_D = \frac{\langle P_{2n}\rangle_I}{\langle P_{2n}\rangle_{I^m}}.$$

Now, a sharp reflection at angle α_0 to the molecular axis gives

$$\langle P_{2n}\rangle_{I^m} = P_{2n}(\cos\alpha_0)$$

and therefore the orientation parameters are given by

$$\langle P_{2n}\rangle_D = \frac{\langle P_{2n}\rangle_I}{P_{2n}(\cos\alpha_0)}. \qquad (2)$$

For the special cases $\alpha_0 = 0$ or $\alpha_0 = \pi/2$ this becomes

Meridional reflection ($\alpha_0 = 0$): $\langle P_{2n}\rangle_D = \langle P_{2n}\rangle_I$;

Equatorial reflection ($\alpha_0 = \pi/2$):

$$\langle P_{2n}\rangle_D = \frac{(-1)^n 2^{2n}(n!)^2}{(2n)!} \langle P_{2n}\rangle_I.$$

0567-7394/81/010135-03$01.00