

and in this way the M/m transformations that left the special position invariant could be identified.

Now the β_{ij} (constituting a second-order tensor) transform as follows:

$$\beta'_i{}^j = \sum_{k=1}^3 \sum_{l=1}^3 R_{ik} R_{jl} \beta_{kl}, \quad (2)$$

the matrices R being identical with those in (1). An arbitrary symmetric tensor β was subsequently subjected to the M/m transformations (2), employing the M/m matrices R that left the atomic position invariant. The invariant tensor β_{inv} that displays the desired β -restrictions was then constructed by an application of Wigner's theorem (Wigner, 1931):

$$(\beta_{\text{inv}})_{ij} = \sum_{s=1}^{M/m} (\beta'_s)_{ij}, \quad (3)$$

stating that the invariant tensor can be obtained by a simple summation over the corresponding elements of the sym-

metry-equivalent, arbitrary tensors of the coinciding atoms*. Finally the nature of the invariant tensor was analyzed by a comparison with the 18 tensors of Table 1, a built-in check insuring that no other cases presented themselves.

References

- CRUICKSHANK, D. W. J. (1961). In *Computing Methods and the Phase Problem*. Oxford: Pergamon Press.
International Tables for X-ray Crystallography (1952). Vol. I. Birmingham: Kynoch Press.
 LEVY, H. (1956). *Acta Cryst.* **9**, 679.
 WIGNER, E. (1931). *Gruppentheorie*. Braunschweig.

* A trivial application of Wigner's theorem is the derivation of coordinates of special positions (first-order tensor components) by a summation over the coordinates of certain general positions.

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Triple fault in face-centred cubic crystals. By RYOITIRO SATO, *Central Research Laboratory, Mitsubishi Metal Mining Co., Ltd, Omiya City, Saitama Prefecture, Japan*

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The face-centred cubic structure [Fig. 1(a)] may contain various types of faults in stacking of the close-packed atomic layers (111). In Fig. 1(b), (c), and (d) three examples of such stacking faults are illustrated: the 'single (or intrinsic) fault', the 'double (or extrinsic) fault', and the 'triple fault'. The diffraction theories of the first two were given by Paterson

(1952) and by Johnson (1963) and Warren (1963), respectively. The last one is dealt with in the present paper.

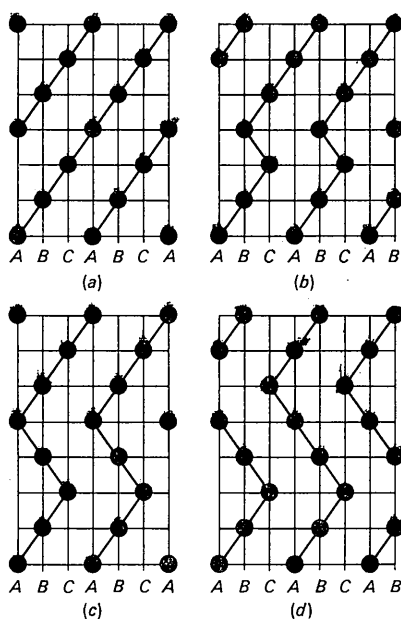


Fig. 1. (a) The unit-layer stacking in the face-centred cubic structure. (b), (c), and (d) contain a single fault, a double fault, and a triple fault, respectively. The horizontal lines are the sections of the unit-layers.

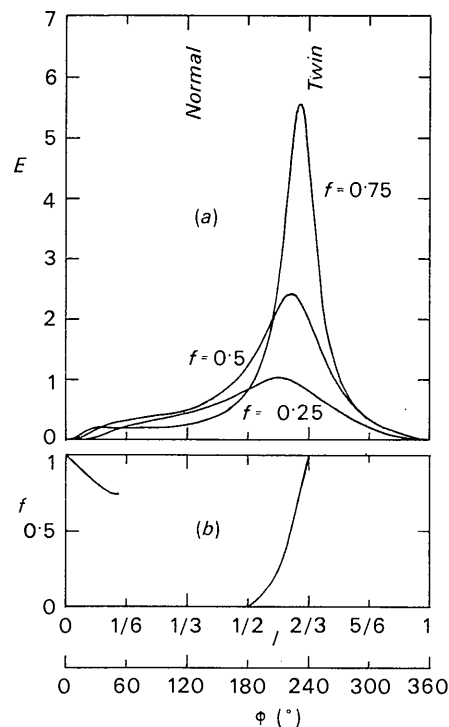


Fig. 2. (a) The function E for $h-k=1 \pmod{3}$ for various values of f . The curves for $h-k=-1 \pmod{3}$ are obtained by replacing l by $-l$. (b) Change in peak position of E in (a) as a function of f . $\phi = 360^\circ \times l$.

In a crystal containing triple faults [Fig. 1(d)], all the layers except for the paired layers at each fault occupy the regular sites, and the order of the sites of the paired layers is reversed compared with the regular stacking. Because of this characteristic nature, the triple fault may be of importance in some physical processes. For instance, Jagodzinski (1954) pointed out that for the cubic-hexagonal transformation of zinc sulphide such triple faults, which are presumably caused by 'doppelte Drehversetzung', are necessary.

For discussion of diffraction by such disordered crystals, it is convenient to use the unit-layer hexagonal indices $hk \cdot l$, which are related to the cubic indices HKL as follows:

$$\begin{aligned} h &= -H/2 + K/2 \\ k &= -K/2 + L/2 \\ l &= H/3 + K/3 + L/3. \end{aligned}$$

As is well known, diffraction effects of such stacking faults appear only on the reciprocal lines $h-k = \pm 1 \pmod{3}$.

The mathematics in the present case can readily be handled by the usual difference equation method (Wilson, 1942). If the number N of layers is assumed to be sufficiently large, the intensity I on the lines $h-k = \pm 1 \pmod{3}$ as a function of continuous-valued l is calculated to be

$$I = (1-f)^2 \frac{\sin^2 N\pi(l \mp \frac{1}{3})}{\sin^2 \pi(l \mp \frac{1}{3})} + NE, \\ E = 6f(1-f)(3-2f) \times \left\{ \frac{1 - \cos 2\pi l}{9 - 18f + 10f^2 + 2f(3-f) \cos 2\pi(l \mp \frac{1}{3}) + 4f(3-2f) \cos^2 2\pi(l \mp \frac{1}{3})} \right\},$$

where f is the fraction of the 'twinned' layers, which is related to the triple-fault probability γ as $f = 3\gamma/(1+2\gamma)$. The first term of the equation for I gives the sharp reflexions

based on the above-mentioned characteristic nature of the triple fault; this term is no more than the usual interference function with its principal maxima at the 'normal' positions, but with the coefficient $(1-f)^2$ of a reasonable form. The second term NE gives the diffuse reflexions due to the faults. As is seen in Fig. 2, the main peak of the function E becomes sharper and higher and approaches to the 'twin' position, as f increases. Another peak appears in E for large values of f , but it is very weak. It is remarkable that E vanishes invariably at $l=0 \pmod{3}$.

It should be noted that, for $f=\gamma=0$, I turns into the interference function with its principal maxima at the 'normal' positions. For $f=\gamma=1$, on the other hand, I vanishes. For this paradox the above assumption regarding N is responsible. When the higher terms which have been neglected on this assumption for obtaining I are taken into account, the interference function with its principal maxima at the 'twin' positions can duly be obtained for $f=\gamma=1$.

References

- JAGODZINSKI, H. (1954). *Neues Jb. Miner., Mh.* **10**, 200.
 JOHNSON, C. A. (1963). *Acta Cryst.* **16**, 490.
 PATERSON, M. S. (1952). *J. Appl. Phys.* **23**, 805.
 WARREN, B. E. (1963). *J. Appl. Phys.* **34**, 1973.
 WILSON, A. J. C. (1942). *Proc. Roy. Soc. A*, **180**, 277.

Books Received

The following books have been received by the Editor. Brief and generally uncritical notices are given of works of marginal crystallographic interest; occasionally a book of fundamental interest is included under this heading because of difficulty in finding a suitable reviewer without great delay. Mention here does not necessarily preclude a full review at a later date.

Les matériaux semi-conducteurs. BY M. RODOT. Pp. xiv + 288. Paris: Dunod, 1965. Price 37 F.

This is the second of a series of monographs on electronic subjects. After a review of the properties and composition of semi-conducting materials it contains chapters on structure defects, relations between the concentrations of imperfections, preparation and testing of crystals, band structure, relaxation mechanisms, properties of principal semi-conductors, special semi-conductors, and closes with a review of their applications. Among the tables at the end of the book is one giving the structure types and cell dimensions of many materials. There is no index, but a fairly extensive table of contents. It will be found a very useful introduction.

Principles of zoological micropalaeontology. Volume 2. BY VLADIMÍR POKORNÝ. Pp. x + 465. Oxford: Pergamon Press, 1965. Price 80 s.

The applications of this attractive and well-illustrated book are geological, zoological, and practical (discovery of oil), rather than crystallographic.

Théorie mathématique de la diffractométrie des poudres aux rayons X. PAR A. J. C. WILSON. Pp. ix + 131. Eindhoven: Editions Centrex (Bibliothèque Technique Philips), 1964.

L'édition anglaise parut en 1963 (*Acta Cryst.* **17**, 791, 1964). On donne en détail l'effet des facteurs géométriques sur les centroïdes et moyennes quadratiques des raies dans les chapitres II-V, ainsi que les résultats correspondant aux positions des sommets et aux largeurs intégrales chaque fois que possible. Les limites inévitables imposées par la nature du rayonnement X et son interaction avec la matière sont étudiées dans le chapitre VI, et on donne un interprétation des effets des imperfections cristallines dans les chapitres VIII et IX.

Interprétation géochimique des éléments en traces dans les roches cristallines. BY DENIS M. SHAW. Pp. vii + 234. Paris: Masson, 1964. Price 56 F.

The author is Professor of Geology at McMaster University, Hamilton, Canada. He spent the academic year 1959-1960 (title page) or 1961-1962 (preface) in Nancy, and this book