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Double fault in hexagonal close-packed crystals. By RYOITIRO SATO, *Central Research Laboratory, Mitsubishi Metal Mining Co., Ltd., Omiya City, Saitama Prefecture, Japan*

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The triple fault in f.c.c. and the double fault in h.c.p. crystals are stacking faults of the type in which changes in sites of unit layers occur only at faults. The diffraction theory of the latter fault is dealt with on the basis of the matrix method.

As pointed out previously by the present author (Sato, 1966), the sites of close-packed atomic layers outside a *triple* fault in f.c.c. crystals are not affected by its presence at all. This remarkable feature is also seen in the *double* fault in h.c.p. crystals, which is formed when a *single* fault [Fig. 1, (a) or (a')] (Christian, 1954) is immediately followed by another *single* fault. The feature concerned is illustrated in Fig. 1, (b) or (b'). Thus the *double* fault in h.c.p. and the *triple* fault in f.c.c. crystals correspond to *einfache* and *doppelte* 'Drehversetzungen' respectively, discussed by Jagodzinski (1954).

For the present problem it is convenient to adopt the unit-layer hexagonal indices $hk.\zeta$, which are related to the ordinary hexagonal indices $hk.l$ as $\zeta = l/2$. As is well known, diffraction effects of stacking faults appear only along the reciprocal lines $h-k \neq 0 \pmod{3}$. The relative intensity I on these lines as a function of continuous-valued ζ is readily calculated by the matrix method given by Kakinoki (1965, 1967) and Kakinoki & Komura (1965). The first procedure in this method is to tabulate the probabilities for occurrences of all kinds of layers. If, in the starting crystal, the sequence of an A , B , or C layer to the subsequent layer is

positive (or negative), the suffix 1 (or 2) will be attached to A , B , or C . The terms positive and negative denote the sequences $A \rightarrow B \rightarrow C \rightarrow A$ and $A \rightarrow C \rightarrow B \rightarrow A$, respectively (*International Tables for X-Ray Crystallography*, 1959). If, furthermore, the sequence of a layer to the subsequent one is governed by the probability of unity, a prime will be attached. Then, the table required is given as follows:

	A_1 A_2 A'_1 A'_2	B_1 B_2 B'_1 B'_2	C_1 C_2 C'_1 C_2
A_1			
A_2		1	β
A'_1			
A'_2		β	1
B_1	β		
B_2		1	$1-\beta$
B'_1			
B'_2	$1-\beta$		β
C_1		$1-\beta$	
C_2	1	β	
C'_1			
C'_2	β	$1-\beta$	1

where β is the double-fault probability and the values at the blanks are all 0.

If the number N of unit layers is assumed to be sufficiently large, the final result is

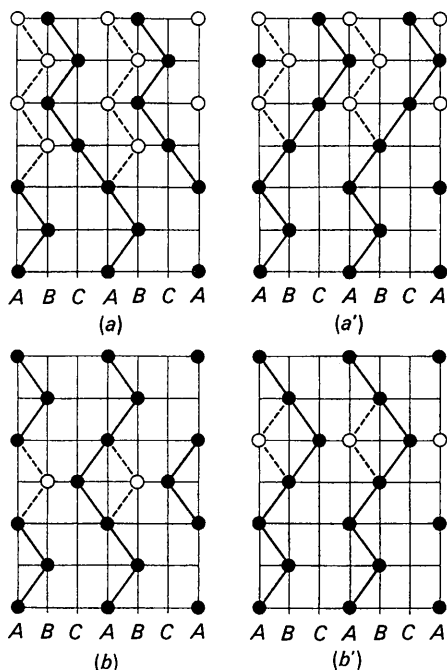


Fig. 1. Unit-layer stackings in the h.c.p. structure containing a *single* fault [(a) and (a')] and a *double* fault [(b) and (b')]. The horizontal lines are the sections of the unit layers. Open circles and broken lines indicate the zigzag characteristic to the starting h.c.p. structure.

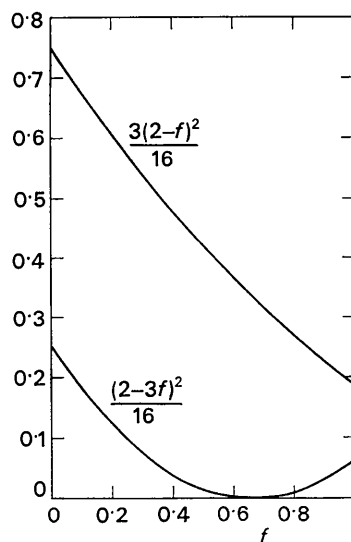


Fig. 2. The coefficients in the first two terms of the equation for I versus f .

$$I = \frac{(2-3f)^2}{16} \frac{\sin^2 N\pi\zeta}{\sin^2 \pi\zeta} + \frac{3(2-f)^2}{16} \frac{\sin^2 N\pi(\zeta - \frac{1}{2})}{\sin^2 \pi(\zeta - \frac{1}{2})} + NE,$$

$$E = \frac{1}{2} f(1-f)(2-f) \left\{ \frac{1}{2-f(2-f)(1+\cos 2\pi\zeta)} \right\} + \frac{3}{2-f(2-f)(1-\cos 2\pi\zeta)}$$

where f is the fraction of 'twinned' two-layer sequences, which is related to β as $f=2\beta/(1+\beta)$.

The first and second terms of the equation for I give the sharp reflexions due to the above remarkable feature of the double fault; each of them is the Laue function having the principal maxima at $\zeta=0$ or $\frac{1}{2}$ mod 1, but with a coefficient involving f . The two coefficients are plotted in Fig. 2 against f . The last term NE gives the diffuse reflexions due to the faults. As is seen in Fig. 3, the peaks of the function E become sharper and higher as f increases. Peak displacement does not occur in any case.

For $f=\beta=0$, I gives duly the diffraction from the starting h.c.p. crystal; the coefficients in the first and second terms become $\frac{1}{2}$ and $\frac{3}{2}$, respectively, and E vanishes. The crystal for $f=\beta=1$ is the twin, as a whole, of the starting crystal, which should give rise to the diffraction same as that of the starting crystal. For $f=\beta=1$, however, the two coefficients become $\frac{1}{6}$ and $\frac{3}{6}$, respectively, although E duly vanishes. This discrepancy is ascribed to the above assumption regarding N . When the higher terms which have been neglected on this assumption for obtaining I are taken into account, the same reflexions as those for $f=\beta=0$ can duly be obtained for $f=\beta=1$.

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Phasenbeziehungen des tetragonalen Kristallsystems. Von ERNST SCHULTZE-RHONHOF, *Anorganisch-Chemisches Institut der Universität, 53 Bonn, Meckenheimer Allee 168, Deutschland*

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Attention is drawn to phase relations of reflexions in tetragonal space groups missing from *International Tables for X-ray Crystallography*.

Im tetragonalen System kann man einer Netzebene (hkl) weitere 15 Ebenen zuordnen, deren Indices sich aus den Indices (hkl) durch Anwendung einer Gruppe von Operationen erzeugen lassen. Diese Operationen sind:

(a) Vorzeichenänderung von h , k und l , entsprechend Spiegelungen an den Ebenen $0kl$, $h0l$ und $hk0$ im reziproken Gitter, und

(b) Vertauschen der Indices h und k , entsprechend einer Spiegelung an der Ebene hhl .

Die Strukturamplituden $|F(hkl)|$ und Phasen $\alpha(hkl)$ dieser 16 Netzebenen sind durch Gesetzmäßigkeiten verknüpft, die bisher nur für diejenigen Flächen tabelliert sind, die durch Anwendung der Untergruppe (a) auseinander hervorgehen (*International Tables for X-ray Crystallography*, 1952). Diese Arbeit, die in Reihenfolge und Aufstellung der einzelnen Raumgruppen den *International Tables* (1952)

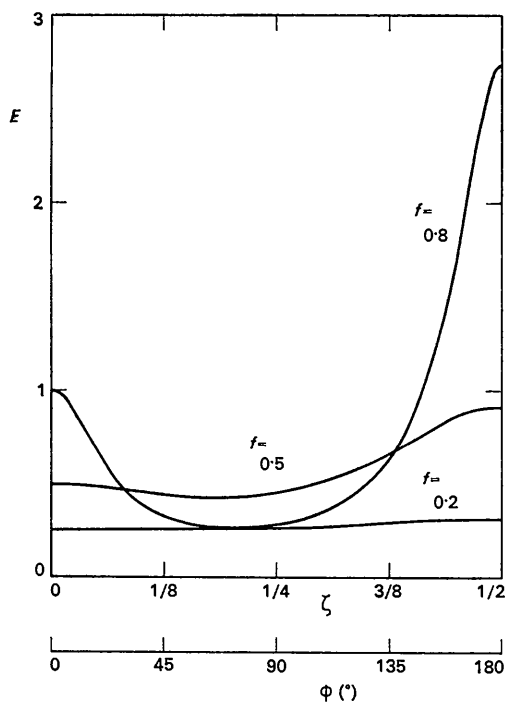


Fig. 3. The function E for various values of f . The curves are symmetric with respect to $\zeta=0$ and $\frac{1}{2}$. $\phi=360^\circ \times \zeta$.

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folgt, gibt eine Tabelle der fehlenden Zusammenhänge.* Die Formeln wurden für alle möglichen Fälle analytisch berechnet und davon unabhängig auf der IBM 7090 des Rheinisch-Westfälischen Institutes für Instrumentelle Mathematik, Bonn, nachgeprüft.

Literatur

- International Tables for X-ray Crystallography* (1952). Vol. I, S. 415 ff. Birmingham: Kynoch Press.

* *Editorial note*: The Table is omitted from this Short Communication because the information which it contains will be included in a complete list of corrections for Vol. I which is being prepared by the Commission on *International Tables*. It is proposed to publish the list in the near future.