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

$$E=\tfrac{1}{8}f(1-f)(2-f)\left\{\frac{1}{2-f(2-f)(1+\cos 2\pi\zeta)}\right\}+\frac{3}{2-f(2-f)(1-\cos 2\pi\zeta)}$$

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 $\frac{1}{4}$ and $\frac{3}{4}$, 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 $\frac{1}{16}$ and $\frac{3}{16}$, respectively, although E duly vanishes. This descrepancy 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 $f=\beta=1$.

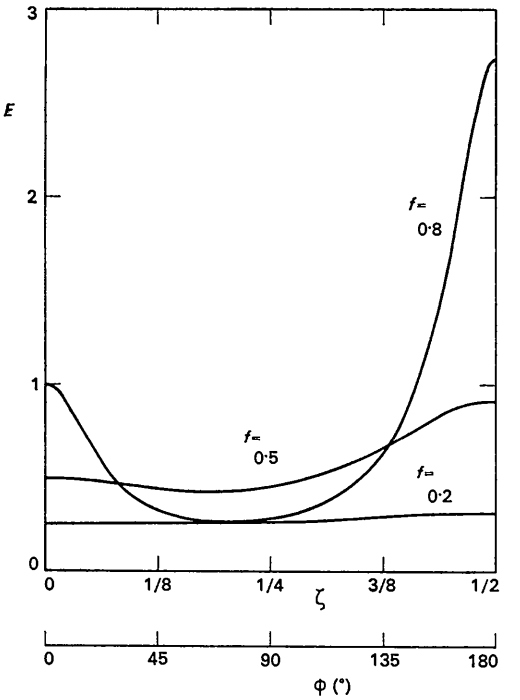

Fig. 3. The function E for various values of f. The curves are symmetric with respect to $\zeta=0$ and $\frac{1}{2}$. $\varphi=360°\times\zeta$.

References

CHRISTIAN, J. W. (1954). *Acta Cryst.* **7**, 415.

International Tables for X-Ray Crystallography (1959). Vol. II, p. 342. Birmingham: Kynoch Press.

JAGODZINSKI, H. (1954). *Neues Jb. Miner., Mh.* **10**, 209.

KAKINOKI, J. (1965). *Nippon Kessyo Gakkwai-Si,* **7**, 66 (in Japanese).

KAKINOKI, J. (1967). *Acta Cryst.* **23**, 875.

KAKINOKI, J. & KOMURA, Y. (1965). *Acta Cryst.* **19**, 137.

SATO, R. (1966). *Acta Cryst.* **20**, 150.

Acta Cryst. (1969). A**25**, 388

Phasenbeziehungen des tetragonalen Kristallsystems.

Von ERNST SCHULTZE-RHONHOF, *Anorganisch-Chemisches Institut der Universität, 53 Bonn, Meckenheimer Allee* 168, *Deutschland*

(*Eingegangen am* 28. *Mai* 1968)

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 0*kl*, *h*0*l* und *hk*0 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) 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.