good apart from some 6·8% of the tetrahedra in the regions where the individual 26-atom clusters pack together.

These results (together with those for α- and β-Mn, also considered as examples) indicate that the coordination polyhedra need not be completely interpenetrating (as in structures such as the Friauf–Laves phases, σ, β-W *etc.*) in order for a structure to achieve an approximation to hypothetical packing of regular tetrahedra to fill space.

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Theory of X-ray Diffraction from Stacking Faults and Antiphase Domain Boundaries in the DO_{19}-Type Ordered H.c.p. Structures

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The mathematical theory of X-ray diffraction from stacking faults and antiphase domain boundaries on the basal plane in the DO_{19}-type ordered hexagonal close-packed structures, exhibited notably by Mg_3Cd and Ti_3Al, has been worked out. In all, seven cases have been considered. There are generally two kinds of diffraction effect obtained, namely the changes in the integrated intensities and the broadening of the reflexions.

Introduction

The first mathematical formulation of the theory of X-ray diffraction from antiphase domain boundaries (APDB's) was carried out by Wilson (1943) (see also Wilson & Zsoldos, 1965) in the ordered face-centred cubic (f.c.c.) structure of the type $L1_2$, a notable example of which is Cu_3Au. Further extensive X-ray work on Cu_3Au has been done by Cohen and his coworkers (see Mikkola & Cohen, 1965, 1966). Rothman, Merion & Cohen (1969) worked out the theory of X-ray diffraction from stacking faults (SF's) and APDB's in the B_2-type body-centred cubic (b.c.c.) structure. In the following is given the theory of SF's and APDB's in another important structure, the hexagonal close-packed (h.c.p.) structure of the type DO_{19}, exhibited notably by Mg_3Cd and Ti_3Al (Fig. 1). After Lele (1969) and Prasad & Lele (1971) the method has been considerably simplified. In general, these 'faults' affect the reflexions in two ways: by changing the integrated intensities and by broadening the reflexions. Reflexions with $H-K=3N$ and $L=2N\pm1$

are absent in both the normal and the superlattice cases. The formulation of the theory is subject to the following assumptions:

(1) The probability of occurrence of 'faults' is small (usually only these values are of physical significance and the assumption obviates consideration of simultaneous occurrence of the faults).

(2) The crystal is infinite and free of distortions.

(3) The scattering power is same for all the close-packed layers.

(4) There is no change in the lattice spacing at the faults.

(5) The faults are distributed at random.

(6) The faults extend over entire domains.

General expression for the diffracted intensity

In terms of the hexagonal basis vectors $\mathbf{A}_1\mathbf{A}_2\mathbf{A}_3$ (double the lattice vectors of the disordered lattice) the position vector of the atom at the (m_1m_2) position in the m_3 layer of a (possibly faulted) h.c.p. crystal (with SF's and APDB's) is given by

$$\mathbf{R}_m = m_1\mathbf{A}_1 + m_2\mathbf{A}_2 + \tfrac{1}{2}m_3\mathbf{A}_3 + \mathbf{r}q_{m_3}\,, \qquad (1)$$

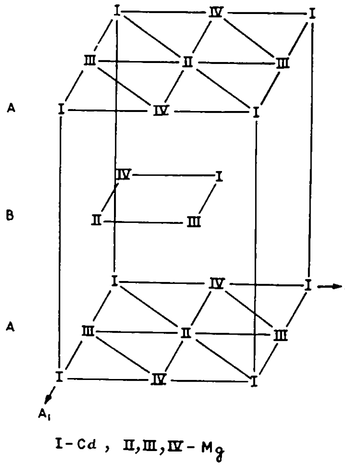

Fig. 1. Unit cell for the ordered h.c.p. DO_{19}-type structure.

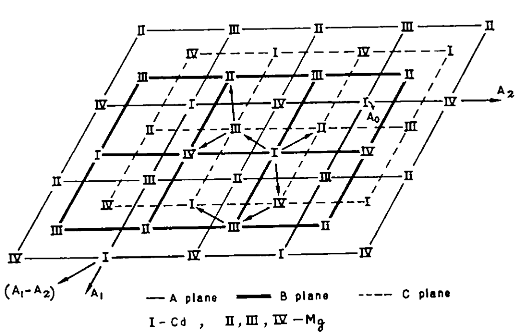

Fig. 2. Basal plane representation of atoms in the three layers A, B, C and the translations of the B layer in its own plane for all the seven kinds of fault.

where $\mathbf{r}$ is the displacement vector given in Table 1 for all the seven types of SF's and APDB's possible on the basal plane and q_{m_3} is a stochastic variable taking the values 0, ± 1, ± 2, *etc.* In Fig. 2 are given the arrangement of the atoms in the basal plane and the various glide vectors. The diffracted intensity from one crystal is given by the usual double sum (Warren, 1969):

$$I(h_1h_2h_3) = I_eF^2 \sum_m \sum_{m'} \exp\left[i2\pi\,\frac{\mathbf{S}-\mathbf{S}_0}{\lambda}\,(\mathbf{R}_m - R_{m'})\right]$$

or

$$I(h_3) = \psi^2 \sum_{m=-\infty}^{+\infty} \exp\,[i\pi m h_3]\langle\exp\,[i\Phi_m]\rangle\,, \qquad (2)$$

where $\mathbf{S}-\mathbf{S}_0/\lambda = h_1\mathbf{B}_1 + h_2\mathbf{B}_2 + h_3\mathbf{B}_3$ and $\mathbf{B}_1\mathbf{B}_2\mathbf{B}_3$ are reciprocal-lattice vectors; ψ^2 is a function of h_1 and h_2, zero everywhere except when $h_1 = H$ and $h_2 = K$, where H and K are integers; Φ_m is the phase difference between the X-rays diffracted from the mth layer and the origin layer and is given by

$$\Phi_m = \frac{2\pi}{\lambda}(\mathbf{S}-\mathbf{S}_0)\,.\,\mathbf{r}(q_{m_3} - q_{m_3^1}) = \frac{2\pi}{\lambda}(\mathbf{S}-\mathbf{S}_0)\,.\,\mathbf{r}q_m$$

and F, the structure factor needs to be evaluated separately for different reflexions (Marcinkowski, 1963).

Table 1. *Displacement vectors for faults*

$\mathbf{r}$	Nature of the fault
$\mathbf{r}_0 = \frac{1}{3}(\mathbf{A}_1 - \mathbf{A}_2)$	—
$\mathbf{r}_1 = \frac{1}{6}(\mathbf{A}_1 - \mathbf{A}_2)$	SF+APDB
$\mathbf{r}_2 = \frac{1}{6}(\mathbf{A}_1 + 2\mathbf{A}_2)$	SF+APDB
$\mathbf{r}_3 = \frac{1}{6}(2\mathbf{A}_1 + \mathbf{A}_2)$	SF+APDB
$\mathbf{r}_4 = -\frac{1}{6}(\mathbf{A}_1 - \mathbf{A}_2)$	APDB
$\mathbf{r}_5 = -\frac{1}{6}(\mathbf{A}_1 + 2\mathbf{A}_2)$	APDB
$\mathbf{r}_6 = \frac{1}{6}(2\mathbf{A}_1 + \mathbf{A}_2)$	APDB
$\mathbf{r}_7 = -\frac{1}{3}(\mathbf{A}_1 - \mathbf{A}_2)$	SF

It is evident that the problem of determining the diffracted intensity reduces to finding the values of $\langle\exp\,[i\Phi_m]\rangle$ in equation (2). Now this can be expressed as

$$\langle\exp\,[i\Phi_m]\rangle = \sum_m P(\Phi_m)\exp\,[i\Phi_m] = \sum_m P(m)\exp\,[i\Phi_m] \qquad (3)$$

where $P(\Phi_m)$ or $P(m)$ is the probability of obtaining the phase difference Φ_m or of arriving at a layer m with the phase difference Φ_m. Fig. 3 shows the probability tree for an $(m-1)$-to-m layer transition with the A_0 type layer at the $(m-1)$ position.

As can be seen, we can have at the $(m-1)$ position any one of the four types of layer A_0, B_1, X_0' and X_1' where X_0' and X_1' denote any of the primed layers, singly or multiply primed. The layers are primed when after a fault the layer does not move into any of the three normal layer positions A, B, C. After a fault all the layers are primed, which can be easily visualized from Fig. 2. But again after a fault of the same kind among the primed layers we are back with the unprimed layer. This is basic to our formulation of the problem. In Fig. 4 is given a complete set of probability trees for the case of SF+APDB of type 1 with the displacement vector $\mathbf{r}_1$.

From these probability trees we can write down a set of difference equations in probabilities $P(m,j)$ and $P'(m,j)$ where m denotes the layer position and j the layer type, 0 or 1.

$$\left.\begin{aligned} P(m,0) &= (1-\alpha_1)P(m-1,1)+\alpha_1 P'(m-1,1) \\ P(m,1) &= (1-\alpha_1)P(m-1,0)+\alpha_1 P'(m-1,0) \\ P'(m,0) &= (1-\alpha_1)P'(m-1,1)+\alpha_1 P(m-1,1) \\ P'(m,1) &= (1-\alpha_1)P'(m-1,0)+\alpha_1 P(m-1,0) \end{aligned}\right\} . \quad (4)$$

Now if equation (3) is written as

$$\langle \exp[i\Phi_m]\rangle = J(m,j) = \sum_{j=0,1} P(m,j)\exp[i\Phi_m]_j , \quad (5)$$

we can get a set of difference equations in $J(m,j)$ and $J'(m,j)$ with the help of the Table 1 for r values and equations (4):

$$\left.\begin{aligned} J(m,0) &= (1-\alpha_1)J(m-1,1)\exp\left[-i\frac{2\pi}{3}(H-K)\right] \\ &\quad +\alpha_1 J'(m-1,1)\exp\left[-i\frac{2\pi}{6}(H-K)\right] \\ J(m,1) &= (1-\alpha_1)J(m-1,0)\exp\left[i\,\frac{2\pi}{3}(H-K)\right] \\ &\quad +\alpha_1 J'(m-1,0)\exp\left[i\,\frac{2\pi}{6}(H-K)\right] \\ J'(m,0) &= (1-\alpha_1)J'(m-1,1)\exp\left[-i\frac{2\pi}{3}(H-K)\right] \\ &\quad +\alpha_1 J(m-1,1)\exp\left[-i\frac{2\pi}{6}(H-K)\right] \\ J'(m,1) &= (1-\alpha_1)J'(m-1,0)\exp\left[i\,\frac{2\pi}{3}(H-K)\right] \\ &\quad +\alpha_1 J(m-1,0)\exp\left[i\,\frac{2\pi}{6}(H-K)\right] \end{aligned}\right\} . \quad (6)$$

If ϱ is the solution of this set of equations, then writing

$$J(m,j) = C_j\varrho^m \quad \text{and} \quad J'(m,j) = C'_j\varrho^m ,$$

we get from equation (6) for non-trivial values of the C's:

$$\begin{vmatrix} \varrho & 0 & -(1-\alpha_1)\varepsilon^{*2} & -\alpha_1\varepsilon^* \\ -(1-\alpha_1)\varepsilon^2 & -\alpha_1\varepsilon & \varrho & 0 \\ 0 & \varrho & -\alpha_1\varepsilon^* & -(1-\alpha_1)\varepsilon^{*2} \\ -\alpha_1\varepsilon & -(1-\alpha_1)\varepsilon^2 & 0 & \varrho \end{vmatrix} = 0 \quad (7)$$

where $\varepsilon = \exp\left[+i\frac{2\pi}{6}(H-K)\right]$.

Expanding the determinant, we get from equation (7):

$$\varrho^4 - 2\varrho^2[\alpha_1^2 + (1-\alpha_1)^2] + (1 - 4\,\alpha_1 + 6\alpha_1^2) - 2\alpha_1^2\cos\frac{2\pi}{3}(H-K) = 0 . \quad (8)$$

Equation (8) has the following four solutions:

Case 1:

$$H-K=3N,\ \cos\frac{2\pi}{3}(H-K)=1$$

$$\varrho_0=1, \varrho_1=-1, \varrho_2=(1-2\alpha_1), \varrho_3=-(1-2\alpha_1) . \quad (9)$$

Case 2:

$$H-K\neq, \quad \cos\ \frac{2\pi}{3}(H-K)=-\tfrac{1}{2}$$

$$\left.\begin{aligned} \varrho_0=(1-\tfrac{1}{2}\alpha_1), \varrho_1=-(1-\tfrac{1}{2}\alpha_1) \\ \varrho_2=(1-\tfrac{3}{2}\alpha_1), \varrho_3=-(1-\tfrac{3}{2}\alpha_1) \end{aligned}\right\} . \quad (10)$$

Higher powers in α_1 are neglected. The same solutions are obtained for the $\mathbf{r}_2$ and $\mathbf{r}_3$ cases as well. While for the $\mathbf{r}_4$, $\mathbf{r}_5$ and $\mathbf{r}_6$ cases the solutions are

$$\varrho_0=1, \varrho_1=-1, \varrho_2=(1-2\alpha), \varrho_3=-(1-2\alpha) . \quad (11)$$

The last case of the displacement vector $\mathbf{r}_7$ is similar to the deformation faults in the disordered case and, after

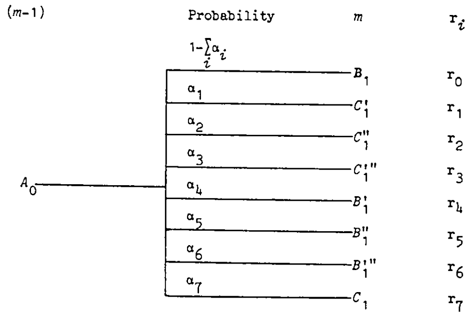

Fig. 3. Probability tree for an $(m-1)$-to-m layer transition.

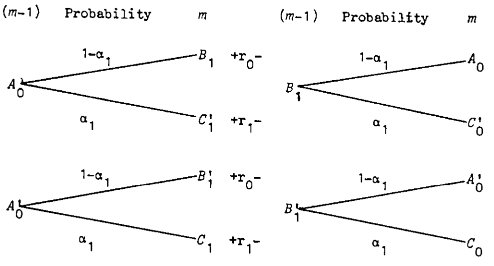

Fig. 4. Probability trees for SF+APDB of type 1.

Warren (1969), the solutions of the characteristic equation for them can be written down as

$$\varrho_0=(1-\tfrac{3}{2}\alpha_7), \quad \varrho_1=-(1-\tfrac{3}{2}\alpha_7)\,. \tag{12}$$

Continuing with our analysis of the $\mathbf{r}_1$ case we now express $\langle\exp[i\Phi_m]\rangle$ in terms of the ϱ's as

$$\langle\exp[i\Phi_m]\rangle=\sum_v C_v\varrho_v^m, \quad v=0,1,2,3\,, \tag{13}$$

where $C_v=C_v^{A_0}+C_v^{B_1}+C_v^{A'_0}+C_v^{B'_1}$ are constants which can be determined if we know the initial conditions for $\langle\exp[i\Phi_m]\rangle$ for $m=0,1,2,3$ and also the probabilities of occurrence of the four types of layers at the origin. If W_0, W_1, W'_0, W'_1 are these probabilities then from Fig. 4 we can write

$$\left.\begin{aligned} W_0&=(1-\alpha_1)W_1+\alpha_1W'_1\\ W_1&=(1-\alpha_1)W_0+\alpha_1W'_0\\ W'_0&=(1-\alpha_1)W'_1+\alpha_1W_1\\ W'_1&=(1-\alpha_1)W'_0+\alpha_1W_0\\ W_0&+W'_0+W_1+W'_1=1 \end{aligned}\right\}\,. \tag{14}$$

These equations yield:

$$W_0=W'_0=W_1=W'_1=\tfrac{1}{4}\,. \tag{15}$$

Following Fig. 4, we can write a four-layer sequence beginning with the four types of layers. From these we get the following four initial conditions:

$$\begin{aligned} J_0&=\langle\exp[i\Phi_0]\rangle=1\\ J_1&=\langle\exp[i\Phi_1]\rangle=(1-\alpha_1)\cos\frac{2\pi}{3}(H-K)\\ &\qquad+\alpha_1\cos\frac{2\pi}{6}(H-K)\\ J_2&=\langle\exp[i\Phi_2]\rangle=(1-2\alpha_1)+2\alpha_1\cos\frac{2\pi}{6}(H-K)\\ J_3&=\langle\exp[i\Phi_3]\rangle=(1-3\alpha_1)\cos\frac{2\pi}{3}(H-K)\\ &\qquad+2\alpha_1\cos\frac{2\pi}{6}(H-K)+\alpha_1\cos\pi(H-K)\,. \end{aligned} \tag{16}$$

In a similar fashion the J's can be found for all other cases. For each reflexion of the type $H-K=3N$ or $3N\pm1$ the values of the J's are same but with added restrictions on the values which H and K take, these being different for different cases. These are:

Case 1: $H-K=3N$

For these reflexions we have the following two sub-cases with further restrictions on the values of H and K as given for each case:

(*a*) (i) $\mathbf{r}_1$ and $\mathbf{r}_4$: N even; (ii) $\mathbf{r}_2$ and $\mathbf{r}_5$: $H+2K=6M$
(iii) $\mathbf{r}_3$ and $\mathbf{r}_6$: $2H+K=6M$
(iv) $\mathbf{r}_7$: this fault does not affect these reflexions.

The J's are:

$$J_0=J_1=J_2=J_3=1\,. \tag{17}$$

The constants C are given by

$$C_0=1, C_1=C_2=C_3=0\,. \tag{18}$$

(*b*) (i) $\mathbf{r}_1$ and $\mathbf{r}_4$: N odd;
(ii) $\mathbf{r}_2$ and $\mathbf{r}_5$: $H+2K=6M\pm3$
(iii) $\mathbf{r}_3$ and $\mathbf{r}_6$: $2H+K=6M\pm3$
(iv) $\mathbf{r}_7$: this fault does not affect these reflexions.

The J's are:

$$\left.\begin{aligned} &J_0=1, J_1=1-2\alpha\,,\\ &J_2=1-4\alpha, J_3=1-6\alpha \end{aligned}\right\} \tag{19}$$

The constants C are given by

$$C_0=C_1=C_3=0, C_2=1\,. \tag{20}$$

Case 2: $H-K=3N\pm1$

Further restrictions on the H and K values give the following sub-cases:

(*a*) (i) $\mathbf{r}_1$: N even; (ii) $\mathbf{r}_2$: $H+2K=6M\pm1$
(iii) $\mathbf{r}_3$: $2H+K=6M\pm1$.

The J's are:

$$\left.\begin{aligned} &J_0=1, J_1=-\tfrac{1}{2}(1-2\alpha)\\ &J_2=(1-\alpha), J_3=-\tfrac{1}{2}(1-3\alpha)\,. \end{aligned}\right\} \tag{21}$$

The constants C are:

$$\left.\begin{aligned} &C_0=\tfrac{1}{4}(1+\tfrac{3}{2}\alpha), \quad C_1=\tfrac{3}{4}(1-\tfrac{1}{2}\alpha)\\ &C_2=C_3=0\,. \end{aligned}\right\} \tag{22}$$

(*b*) (i) $\mathbf{r}_1$: N odd; (ii) $\mathbf{r}_2$: $H+2K=6N\pm4$
(iii) $\mathbf{r}_3$: $2H+K=6M\pm4$.

The J's are:

$$\left.\begin{aligned} &J_0=1, J_1=-\tfrac{1}{2}\\ &J_2=(1-3\alpha), J_3=-\tfrac{1}{2}(1-3\alpha) \end{aligned}\right\}\,. \tag{23}$$

The constants C are:

$$C_0=C_1=0, C_2=\tfrac{1}{4}, C_3=\tfrac{3}{4}\,. \tag{24}$$

(*c*) (i) $\mathbf{r}_4$: N even; (ii) $\mathbf{r}_5$: $H+2K=6M\pm1$
(iii) $\mathbf{r}_6$: $2H+K=6m\pm1$.

The J's are:

$$\left.\begin{aligned} &J_0=1, J_1=-\tfrac{1}{2}(1-2\alpha)\\ &J_2=(1-4\alpha), J_3=-\tfrac{1}{2}(1-6\alpha) \end{aligned}\right\}\,. \tag{25}$$

The constants C are:

$$C_0=C_1=0, C_2=\tfrac{1}{4}, C_3=\tfrac{3}{4}\,. \tag{26}$$

(*d*) (i) $\mathbf{r}_4$: N odd; (ii) $\mathbf{r}_5$: $H+2K=6M\pm4$
(iii) $\mathbf{r}_6$: $2H+K=6M\pm4$.

The J's are:

$$\left.\begin{aligned} &J_0=1, J_1=-\tfrac{1}{2}\\ &J_2=1, J_3=-\tfrac{1}{2}\,. \end{aligned}\right\} \tag{27}$$

The constants C are:

$$C_0=\tfrac{1}{4}, C_1=\tfrac{3}{4}, C_2=C_3=0\,. \tag{28}$$

(e) $\mathbf{r}_7$: The J's are:

$$J_0=1, J_1=-\tfrac{1}{2}\,. \tag{29}$$

The constants C are:

$$C_0=\tfrac{1}{4}(1-\tfrac{3}{2}\alpha)\,,\quad C_1=\tfrac{3}{4}(1+\tfrac{1}{2}\alpha)\,. \tag{30}$$

Now we can get the value of $\langle\exp[i\Phi_m]\rangle$ from equation (13) by substituting the values of the ϱ's and C's and, rewriting equation (13), we have

$$\langle\exp[i\Phi_m]\rangle=C_0\varrho_0^{|m|}+C_1\varrho_1^{|m|}+C_2\varrho_2^{|m|}+C_3\varrho_3^{|m|},\quad -\infty\le m\le+\infty\,. \tag{31}$$

Substitution of equation (31) in (2) gives the diffracted intensity in reciprocal space:

$$\begin{aligned}I(h_3)=&\,C_0\psi^2\sum\varrho_0^{|m|}\cos[m\pi h_3]\\&+C_1\psi^2\sum(-\varrho_1)^{|m|}\cos[m\pi(h_3-1)]\\&+C_2\psi^2\sum\varrho_2^{|m|}\cos[m\pi h_3]\\&+C_3\psi^2\sum(-\varrho_3)^{|m|}\cos[m\pi(h_3-1)]\,,\\&-\infty\le m\le+\infty\,.\end{aligned} \tag{32}$$

The sine terms cancel in pairs. After the summation has been carried out, the diffracted intensity is given by

$$\begin{aligned}I(h_3)=&\,\psi^2\left[\frac{C_0(1-\varrho_0^2)}{1-2\varrho_0\cos\pi h_3+\varrho_0^2}+\frac{C_2(1-\varrho_2^2)}{1-2\varrho_2\cos\pi h_3+\varrho_2^2}\right]\\&+\psi^2\left[\frac{C_1(1-\varrho_1^2)}{1+2\varrho_1\cos\pi(h_3-1)+\varrho_1^2}\right.\\&\left.+\frac{C_3(1-\varrho_3^2)}{1+2\varrho_3\cos\pi(h_3-1)+\varrho_3^2}\right]\,.\end{aligned} \tag{33}$$

The first two expressions in equation (33) are for reflexions centred at $L=0$ mod 2 and the last two expressions give the intensity centred at $L=1$ mod 2. From these we get the following expressions for integrated intensities (T) and the integral breadths (β).

Integrated intensities

1. $H-K=3N$

With the following further restrictions on the H and K values for the individual cases:

(i) $\mathbf{r}_2$ and $\mathbf{r}_5$: $H+2K=6M$ and $6M\pm3$
(ii) $\mathbf{r}_3$ and $\mathbf{r}_6$: $2H+K=6M$ and $6M\pm3$

$$\left.\begin{array}{ll}T_0=2\psi^2\,, & L=0 \text{ mod } 2\\ T_1=0\quad, & L=1 \text{ mod } 2\end{array}\right\}. \tag{34}$$

2. $H-K=3N\pm1$

Further restrictions on the values of H and K give the following cases:

(a) (i) $\mathbf{r}_1$: N even; (ii) $\mathbf{r}_2$: $H+2K=6M\pm1$
(iii) $\mathbf{r}_3$: $2H+K=6M\pm1$

$$\left.\begin{array}{ll}T_0=\tfrac{1}{2}\psi^2(1+\tfrac{3}{2}\alpha)\,, & L=0 \text{ mod } 2\\ T_1=\tfrac{3}{2}\psi^2(1-\tfrac{1}{2}\alpha)\,, & L=1 \text{ mod } 2\end{array}\right\}. \tag{35}$$

(b) (i) $\mathbf{r}_1$: N odd; (ii) $\mathbf{r}_2$: $H+2K=6M\pm4$
(iii) $\mathbf{r}_3$: $2H+K=6M\pm4$
(iv) $\mathbf{r}_5$: $H+2K=6M\pm1$ and $6M\pm4$
(v) $\mathbf{r}_6$: $2H+K=6M\pm1$ and $6M\pm4$

$$\left.\begin{array}{ll}T_0=\tfrac{1}{2}\psi^2\,, & L=0 \text{ mod } 2\\ T_1=\tfrac{3}{2}\psi^2\,, & L=1 \text{ mod } 2\end{array}\right\} \tag{36}$$

(c) $\mathbf{r}_7$:

$$\left.\begin{array}{ll}T_0=\tfrac{1}{2}\psi^2(1-\tfrac{3}{2}\alpha)\,, & L=0 \text{ mod } 2\\ T_1=\tfrac{3}{2}\psi^2(1+\tfrac{1}{2}\alpha)\,, & L=1 \text{ mod } 2\end{array}\right\}. \tag{37}$$

Integral breadths

1. $H-K=3N$

There are the following further restrictions on H and K values for some cases:

(i) $\mathbf{r}_2$ and $\mathbf{r}_5$: $H+2K=6M$ and $6M\pm3$
(ii) $\mathbf{r}_3$ and $\mathbf{r}_6$: $2H+K=6M$ and $6M\pm3$

$$\left.\begin{array}{ll}\beta_0=2\,\alpha, & L=0 \text{ mod } 2\\ \beta_1=0\,, & L=1 \text{ mod } 2\end{array}\right\}. \tag{38}$$

2. $H-K=3N\pm1$

(a) (i) $\mathbf{r}_1$: N even; (ii) $\mathbf{r}_2$: $H+2K=6M\pm1$
(iii) $\mathbf{r}_3$: $2H+K=6M\pm1$

$$\beta=\tfrac{1}{2}\,\alpha,\ L=\text{integer}\,. \tag{39}$$

(b) (i) $\mathbf{r}_1$: N odd; (ii) $\mathbf{r}_2$: $H+2K=6M\pm4$
(iii) $\mathbf{r}_3$: $2H+K=6M\pm4$

$$\beta=\tfrac{3}{2}\alpha\,,\quad L=\text{integer}\,. \tag{40}$$

(c) (i) $\mathbf{r}_5$: $H+2K=6M\pm1$ and $6M\pm4$
(ii) $\mathbf{r}_6$: $2H+K=6M\pm1$ and $6M\pm4$

$$\beta=2\alpha\,,\quad L=\text{integer}\,. \tag{41}$$

(d) $\mathbf{r}_7$:

$$\left.\begin{array}{ll}\beta_0=\tfrac{3}{2}\alpha\,, & L=0 \text{ mod } 2\\ \beta_1=\tfrac{1}{2}\alpha\,, & L=1 \text{ mod } 2\end{array}\right\}. \tag{42}$$

In an actual situation, however, the analysis for all these 'faults' would present some difficulty for two reasons: (i) the presence of small coherently diffracting domains and micro-strains within these and (ii) not enough reflexions being available.

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Statistics of Derived Intensities

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The variance of diffractometer-collected diffraction intensities is discussed in terms of instrumental instability and uncertainties in the parameter used to bring the intensities to a common scale. It is shown that the inconsistent and/or divergent behavior of the reflections used as standards contributes in a major way to the uncertainty in the scaling parameter and can often account for the largest portion of the variance in excess of the Poisson contribution for reflections with large intensities.

Introduction

Intensity data from counter techniques are expected on theoretical grounds to follow the Poisson distribution. They should therefore have variances equal to the total counts in each measurement. It has been found, however, that the variances of the measurements within a crystallographic data set are larger than the measured counts. At least three observations exist which support this statement:

(1) Multiple measurements of intense reflections in a data set agree with each other less well than predicted, if considerable time elapses between measurements;

(2) At convergence of least-squares refinement the observed and calculated data for the more intense reflections disagree more strongly than one might predict using Poisson statistics, and;

(3) the standard error of fit determined from least-squares refinement is usually greater than 1·0 if Poisson statistics variances are used.

Observation 3 is, of course, model dependent while observation 2 is at least potentially model dependent. The largest discrepancies, however, are commonly found among the more intense data. This distribution would seem to have sources other than the model. Many workers (*e.g.*, Busing & Levy, 1957; Peterson & Levy, 1957; Stout & Jensen, 1968, p. 456) have included in the calculation of the variances, S^2, of the intensity data, a term proportional to the square of total counts, T, or net counts, I:

$$e.g.,\ S^2(I)=T+P^2I^2. \qquad (1)$$

The factor P has been termed the 'instability constant' by some workers and the 'ignorance factor' (Corfield, Doedens & Ibers, 1967) by others. It is common practice to use 0·01 to 0·05 for the value of P. The larger values are usually chosen for crystals which show marked decomposition.

Several rationalizations have been advanced for the use of equation (1):

(1) It reduces the weights used for intense reflections in least-squares refinement (but any factor which is an

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