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X-ray Diffraction from Hexagonal Close-Packed Crystals with Deformation Stacking Faults. I. Effect of Solute Segregation at Faults in Alloys

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The Christian–Gevers theory of X-ray diffraction from homogeneous hexagonal close-packed (h.c.p.) crystals with deformation stacking faults is extended to include the effect of segregation of solute atoms at the faults. The results show that the breadths of reflexions remain unaffected by solute segregation. The ratios of integrated intensities of reflexions with $H-K \neq 0$ mod 3, $L=1$ mod 2 and $L=0$ mod 2 respectively are affected, but only to a small extent, that is, within the limits of possible accuracy in experimental measurements of integrated intensity.

Introduction

The theory of X-ray diffraction from h.c.p. crystals with deformation stacking faults on the close-packed planes was first considered by Christian (1954) and Gevers (1954) and subsequently reviewed by Warren (1959). An alternative approach to this problem has recently been given by Lele, Anantharaman & Johnson (1967). These calculations were made under the following assumptions:

(1) The crystal is infinite in size and is free from distortion.

(2) The scattering power is the same for all the close-packed planes.

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

(4) The faults are distributed at random.

(5) The faults extend over entire close-packed planes.

The scattering power for all the close-packed planes is obviously the same for the case of pure metals. For alloys the scattering power of each plane depends on the concentration of the solute in it and should not vary under conditions of thermodynamic equilibrium. However, stacking faults produce localized regions of a different structure and the concentration of the solute atoms may therefore differ from that in the rest of the crystal under equilibrium conditions (Suzuki, 1952). There is thus the possibility of segregation of solute atoms at the stacking faults, and the diffraction effects arising from this segregation to deformation faults in face-centred cubic (f.c.c.) alloys have been described by Willis (1959). The present paper deals with the theory of X-ray diffraction by h.c.p. alloys with deformation stacking faults in which the alloy composition at the fault differs from that of the hexagonal matrix. The calculations have been made under assumptions No. 1 and 3 to 5, listed above.

Fig. 1 illustrates the sequence of close-packed (0002) layers with the faulted positions denoted by F, and f_1 and f_2 represent the scattering powers averaged over the atoms in the two kinds of layer. When several faults occur in succession, the f.c.c. structure is developed only at the boundaries of the set, so that segregation takes place only at the boundaries.

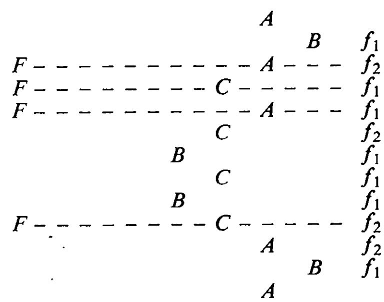

Fig. 1. Stacking sequence of (0002) planes. Faulted positions are denoted by F, and the average scattering powers of the atoms in the two kinds of layer by f_1 and f_2.

Formulation of the problem

We employ ordinary hexagonal axes $\mathbf{A}_1$, $\mathbf{A}_2$ and $\mathbf{A}_3$ ($|\mathbf{A}_3|$ being twice the interlayer spacing), their reciprocal vectors $\mathbf{B}_1$, $\mathbf{B}_2$ and $\mathbf{B}_3$, the hexagonal indices HKL and continuous parameters h_1, h_2 and h_3 such that any vector $\mathbf{S}$ in reciprocal space can be expressed as

$$\mathbf{S}=h_1\mathbf{B}_1+h_2\mathbf{B}_2+h_3\mathbf{B}_3\ .$$

The diffracted intensity is then given by a single summation over all layers (Warren, 1959):

$$I(h_3)=\psi^2 \sum_{m=-\infty}^{\infty} \langle f_{m_3}f_{m'_3}\exp\,[i\Phi_m]\rangle \exp\,[\pi imh_3]\ , \quad (1)$$

where ψ^2 is a function of h_1 and h_2 which vanishes except when $h_1=H$ and $h_2=K$, f_{m_3} and $f_{m'_3}$ are the structure factors of the m_3 and m'_3 layers and Φ_m is the phase difference between X-rays scattered through $H\mathbf{B}_1+K\mathbf{B}_2$ by two layers, m_3 and m'_3, which are m layers apart.

Let P_{11}, P_{12}, P_{21}, P_{22} be the probabilities that layers m_3 and m'_3 respectively have atoms of average scattering power f_1 and f_1, f_1 and f_2, f_2 and f_1, f_2 and f_2 and let $\langle \exp[i\Phi_m]\rangle_{11}$, $\langle \exp[i\Phi_m]\rangle_{12}$, $\langle \exp[i\Phi_m]\rangle_{21}$, $\langle \exp[i\Phi_m]\rangle_{22}$ be the corresponding values of $\langle \exp[i\Phi_m]\rangle$ for all such pairs of layers. Thus

$$\langle f_{m_3} f_{m'_3} \exp[i\Phi_m]\rangle = \sum_{i=1}^{2}\sum_{j=1}^{2} P_{ij} f_i f_j \langle \exp[i\Phi_m]\rangle_{ij} . \quad (2)$$

Introducing

$$\sigma = \frac{(f_1-f_2)}{(f_1+f_2)} = \frac{(f_1-f_2)}{2f} , \quad (3)$$

one obtains

$$\begin{aligned}\langle f_{m_3} f_{m'_3} \exp[i\Phi_m]\rangle = f^2\{&P_{11}\langle \exp[i\Phi_m]\rangle_{11} \\ &+P_{12}\langle \exp[i\Phi_m]\rangle_{12}+P_{21}\langle \exp[i\Phi_m]\rangle_{21} \\ &+P_{22}\langle \exp[i\Phi_m]\rangle_{22}+2\sigma(P_{11}\langle \exp[i\Phi_m]\rangle_{11} \\ &-P_{22}\langle \exp[i\Phi_m]\rangle_{22})+\sigma^2(P_{11}\langle \exp[i\Phi_m]\rangle_{11} \\ &-P_{12}\langle \exp[i\Phi_m]\rangle_{12}-P_{21}\langle \exp[i\Phi_m]\rangle_{21} \\ &+P_{22}\langle \exp[i\Phi_m]\rangle_{22})\} . \quad (4)\end{aligned}$$

In general, Φ_m can be expressed as the sum of the individual phase shifts, φ_k, across successive layers:

$$\Phi_m = \sum_{k=m_3+1}^{m'_3} \varphi_k , \quad (5)$$

where φ_k can take either of the values $+\varphi_0$ and $-\varphi_0$ where $\varphi_0=(2\pi/3)(H-K)$. We wish to compute the expectation values $\langle \exp[i\Phi_m]\rangle_{ij}$ $(i,j=1,2)$ by considering an appropriate random walk in the individual phase differences $\pm\varphi_0$. In this random walk a phase difference $+\varphi_0$ $(-\varphi_0)$ is unaltered with a probability $(1-\alpha)$ and is changed to $-\varphi_0$ $(+\varphi_0)$ with probability α, where α is the deformation fault probability. We choose some particular plane, m_3, as the starting point of the random walk and terminate it at some other plane $m'_3=m_3+m$. Suppose that, counting even and odd planes from the plane m_3, there are k_1 and k_2 faults on even- and odd-numbered planes respectively, then the net phase difference found between the beginning and end of the walk will be

$$\left.\begin{aligned}\Phi_m^A &= +\varphi_0\left[\frac{1-(-1)^m}{2}+k_1-k_2\right] \\ \Phi_m^B &= -\varphi_0\left[\frac{1-(-1)^m}{2}+k_1-k_2\right]\end{aligned}\right\} , \quad (6)$$

depending on whether the initial plane is A or B type. (A plane is of A type if, in the absence of a fault, the phase difference between it and the next succeeding plane is $+\varphi_0$; it is of B type if this phase difference is $-\varphi_0$.) Since $\varphi_{(-i)}=\varphi_{(+i)}$, we also have

$$\Phi^{A,B}_{(-m)} = \Phi^{A,B}_{(+m)} . \quad (7)$$

The probability of obtaining a phase difference Φ_m^A after m steps is just the probability, $P(m,k_1,k_2)$, of obtaining k_1 and k_2 faults on the even- and odd-numbered planes respectively, multiplied by the probability, $P(A)$, of obtaining an A type plane initially:

$$\begin{aligned}P(\Phi^A_{m,k_1,k_2}) &= P(m,k_1,k_2)P(A) \\ &= \frac{1}{2}\cdot\frac{n_1!}{k_1!(n_1-k_1)!}\cdot\frac{n_2!}{k_2!(n_2-k_2)!} \\ &\quad\times \alpha^{k_1+k_2}(1-\alpha)^{m-k_1-k_2} , \quad (8)\end{aligned}$$

where n_1 and n_2 are respectively the number of even- and odd-numbered planes and are given by

$$n_1 = \frac{m}{2} + \tfrac{1}{2}\left[\frac{1-(-1)^m}{2}\right] , \quad (9a)$$

$$n_2 = \frac{m}{2} - \tfrac{1}{2}\left[\frac{1-(-1)^m}{2}\right] . \quad (9b)$$

Calculation of $\langle f_{m_3} f_{m'_3} \exp[i\Phi_m]\rangle$

Three cases arise and we shall consider them in turn. I. $m=0$: considering the sequences in Fig. 2, we obtain, since the mth layer is f_1-type in the first pair of sequences and f_2-type in the last pair:

$$P_{11} = 1-2\alpha(1-\alpha) , \quad (10a)$$

$$P_{12} = P_{21} = 0 , \quad (10b)$$

$$P_{22} = 2\alpha(1-\alpha) . \quad (10c)$$

Since Φ_0 is always equal to zero, we get

$$\langle \exp[i\Phi_0]\rangle_{11} = \langle \exp[i\Phi_0]\rangle_{22} = 1 . \quad (11)$$

Substituting from equations (10) and (11) in equation (4), we have

$$\langle f_{m_3} f_{m'_3} \exp[i\Phi_0]\rangle / f^2 = 1 + \frac{2\sigma}{3}(4\varrho^2-1)+\sigma^2 , \quad (12)$$

where

$$\varrho^2 = 1-3\alpha(1-\alpha) . \quad (13)$$

II. $m=1$: by considering the eight types of stacking sequences illustrated in Fig. 3, we obtain

$$P_{11} = 1-3\alpha(1-\alpha) , \quad (14a)$$

$$P_{12} = P_{21} = P_{22} = \alpha(1-\alpha) . \quad (14b)$$

A. $(H-K)=0$ mod 3. In this case Φ_1 is equal to zero

Layer	1		2		3		4	
+1	A			A		C	B	
0		B	C		B			C
−1	A			A	A			A
	$(1-\alpha)^2$		α^2		$(1-\alpha)\alpha$		$\alpha(1-\alpha)$	

Fig. 2. Different types of stacking sequences for three successive layers and their associated probabilities.

and hence

$$\langle \exp [i\Phi_1]\rangle_{ij} = 1\,, \quad (i,j=1,2) \tag{15}$$

which on substitution in equation (4) yields

$$\langle f_{m_3} f_{m'_3} \exp [i\Phi_1]\rangle / f^2 = 1 + \frac{2\sigma}{3}(4\varrho^2-1) + \frac{\sigma^2}{3}(4\varrho^2-1)\,. \tag{16}$$

B. $(H-K)\neq 0 \bmod 3$. From a consideration of the sequences in Fig. 3, it is clear that Φ_1 takes either of the values $+\varphi_0$ or $-\varphi_0$ with equal probability. Therefore,

$$\langle \exp [i\Phi_1]\rangle_{ij} = -\tfrac{1}{2}\,, \quad (i,j=1,2)\,. \tag{17}$$

Introducing the above values in equation (4), we get

$$\langle f_{m_3} f_{m'_3} \exp [i\Phi_1]\rangle / f^2 = -\tfrac{1}{2}\left[1 + \frac{2\sigma}{3}(4\varrho^2-1) + \frac{\sigma^2}{3}(4\varrho^2-1)\right]. \tag{18}$$

III. $m\geq 2$: it is useful to consider an $(m-2)$ plane sequence numbered from 1 to $(m-1)$. At one end we can now add the zero and -1th planes and at the other the mth and $(m+1)$th. This can be done in any one of the sixteen ways illustrated in Fig. 4 and with the probabilities indicated there. Let the number of faults in the m-layer sequence be k_1+k_2 of which k_1 are on even-numbered planes and k_2 on odd-numbered ones. An $(m-2)$-layer sequence may therefore contain:

(i) (k_1+k_2) faults so that the zero and mth layers are added without introducing further faults;

(ii) (k_1+k_2-1) faults so that the zero layer is added without introducing a further fault but the mth layer is faulted;

(iii) (k_1+k_2-1) faults so that there is a fault between the zero and the 1st layer but none between the $(m-1)$th and mth layers;

(iv) (k_1+k_2-2) faults so that both the zero and mth layers are added with faults.

The probabilities for obtaining the above four distributions of stacking faults in an $(m-2)$-layer sequence are respectively as follows:

(i) $P(m-2,k_2,k_1)$;
(ii) $P(m-2,k_2-1,k_1)$ for m even and $P(m-2,k_2,k_1-1)$ for m odd;
(iii) $P(m-2,k_2,k_1-1)$;
(iv) $P(m-2,k_2-1,k_1-1)$ for m even and $P(m-2,k_2,k_1-2)$ for m odd.

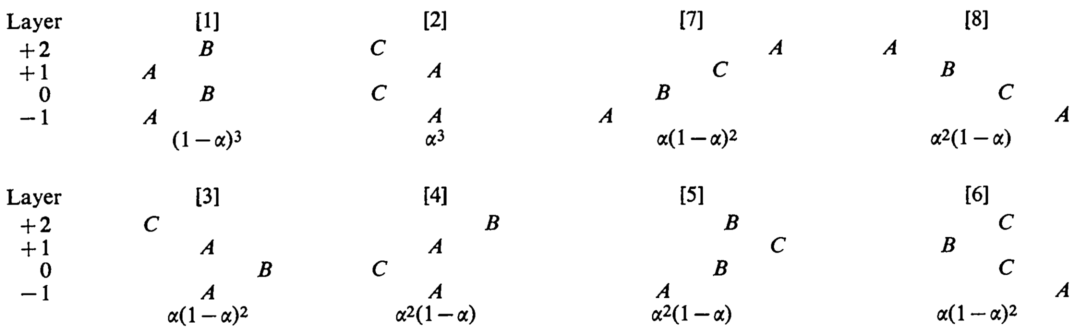

Fig. 3. Different types of stacking sequences for four successive layers and the probabilities for their occurrence.

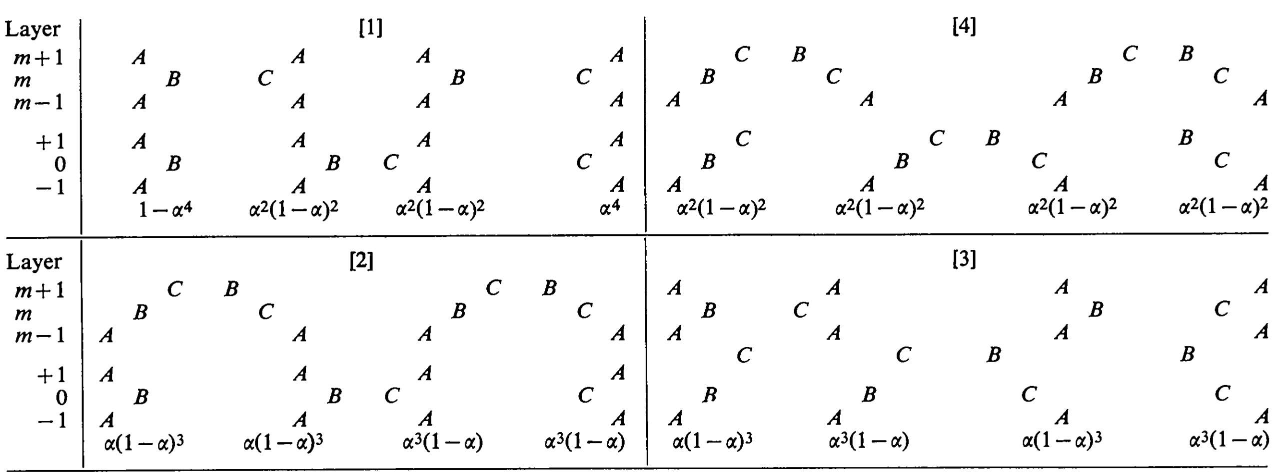

Fig. 4. Different types of sequences for the six layers -1, 0, $+1$, $m-1$, m, $m+1$, where $m\geq 2$, and their probabilities.

The probabilities for adding the zero and mth layers for the above four cases are respectively $(1-\alpha)^2$, $(1-\alpha)\alpha$, $\alpha(1-\alpha)$ and α^2. As a check, it can be easily shown that

$$\left.\begin{aligned} P(m,k_1,k_2)=&(1-\alpha)^2P(m-2,k_2,k_1)\\ &+\alpha(1-\alpha)P(m-2,k_2-1,k_1)\\ &+\alpha(1-\alpha)P(m-2,k_2,k_1-1)\\ &+\alpha^2P(m-2,k_2-1,k_1-1) \text{ for } m \text{ even}\\ =&(1-\alpha)^2P(m-2,k_2,k_1)\\ &+\alpha(1-\alpha)P(m-2,k_2,k_1-1)\\ &+\alpha(1-\alpha)P(m-2,k_2,k_1-1)\\ &+\alpha^2P(m-2,k_2,k_1-2) \text{ for } m \text{ odd}. \end{aligned}\right\} \quad (19)$$

For the first four sequences in Fig. 4, the scattering powers of the zero and mth layers are f_1 and f_1, for the next four sequences f_1 and f_2, for the next four sequences f_2 and f_1 and for the last four sequences f_2 and f_2. Thus

$$P_{11}=(1-\alpha)^4+2\alpha^2(1-\alpha)^2+\alpha^4\,, \quad (20a)$$

$$P_{12}=P_{21}=2\alpha(1-\alpha)^3+2\alpha^3(1-\alpha)\,, \quad (20b)$$

$$P_{22}=4\alpha^2(1-\alpha)^2\,. \quad (20c)$$

A. $(H-K)=0$ mod 3. In this case also Φ_m is equal to zero and consequently

$$\langle \exp[i\Phi_m]\rangle_{ij}=1\,, \quad (i,j=1,2)\,. \quad (21)$$

Substituting the above in equation (4), one obtains

$$\langle f_{m_3}f_{m'_3}\exp[i\Phi_m]\rangle/f^2=\left[1+\frac{\sigma}{3}(4\varrho^2-1)\right]^2.\ m\geq 2 \quad (22)$$

B. $(H-K)\neq 0$ mod 3. A consideration of the four groups of stacking sequences illustrated in Fig. 4 leads to expressions for $P_{ij}\langle\exp[i\Phi_m]\rangle_{ij}$ $(i,j=1,2)$, which can be concisely written in matrix notation as follows:

$$\begin{bmatrix} P_{11}\langle\exp[i\Phi_m]\rangle_{11}\\ P_{12}\langle\exp[i\Phi_m]\rangle_{12}\\ P_{21}\langle\exp[i\Phi_m]\rangle_{21}\\ P_{22}\langle\exp[i\Phi_m]\rangle_{22}\end{bmatrix} = \begin{bmatrix} (1-\alpha)^4 & \alpha^2(1-\alpha)^2 & \alpha^2(1-\alpha)^2 & \alpha^4\\ \alpha(1-\alpha)^3 & \alpha(1-\alpha)^3 & \alpha^3(1-\alpha) & \alpha^3(1-\alpha)\\ \alpha(1-\alpha)^3 & \alpha^3(1-\alpha) & \alpha(1-\alpha)^3 & \alpha^3(1-\alpha)\\ \alpha^2(1-\alpha)^2 & \alpha^2(1-\alpha)^2 & \alpha^2(1-\alpha)^2 & \alpha^2(1-\alpha)^2 \end{bmatrix} \begin{bmatrix} Q_1\\ Q_2\\ Q_3\\ Q_4\end{bmatrix}, \quad (23)$$

where

$$Q_1=\tfrac{1}{2}\,\Sigma\,\Sigma\,P(m-2,k_2,k_1)\,\{\exp[i\Phi^A_{m,k_1,k_2}] + \exp[i\Phi^B_{m,k_1,k_2}]\}\,, \quad (24a)$$

$$\left.\begin{aligned} Q_2=&\tfrac{1}{2}\,\Sigma\,\Sigma\,P(m-2,k_2-1,k_1)\,\{\exp[i\Phi^A_{m,k_1,k_2}]\\ &+\exp[i\Phi^B_{m,k_1,k_2}]\} \text{ for } m \text{ even}\\ =&\tfrac{1}{2}\,\Sigma\,\Sigma\,P(m-2,k_2,k_1-1)\,\{\exp[i\Phi^A_{m,k_1,k_2}]\\ &+\exp[i\Phi^B_{m,k_1,k_2}]\} \text{ for } m \text{ odd} \end{aligned}\right\}, \quad (24b)$$

$$Q_3=\tfrac{1}{2}\,\Sigma\,\Sigma\,P(m-2,k_2,k_1-1)\,\{\exp[i\Phi^A_{m,k_1,k_2}] + \exp[i\Phi^B_{m,k_1,k_2}]\}\,, \quad (24c)$$

$$\left.\begin{aligned} Q_4=&\tfrac{1}{2}\,\Sigma\,\Sigma\,P(m-2,k_2-1,k_1-1)\,\{\exp[i\Phi^A_{m,k_1,k_2}]\\ &+\exp[i\Phi^B_{m,k_1,k_2}]\} \text{ for } m \text{ even}\\ =&\tfrac{1}{2}\,\Sigma\,\Sigma\,P(m-2,k_2,k_1-2)\,\{\exp[i\Phi^A_{m,k_1,k_2}]\\ &+\exp[i\Phi^B_{m,k_1,k_2}]\} \text{ for } m \text{ odd} \end{aligned}\right\}. \quad (24d)$$

Substituting from equations (6) and (8) in the above, simplifying and then inserting the values of Q_1, Q_2, Q_3 and Q_4 in equation (23), we have:

$$P_{11}\langle\exp[i\Phi_m]\rangle_{11}=\frac{\varrho^m}{36\varrho^3}[(2\varrho-1)(1+3\varrho-\varrho^2)^2 +(-1)^m(2\varrho+1)(1-3\varrho-\varrho^2)^2]\,, \quad (25a)$$

$$P_{12}\langle\exp[i\Phi_m]\rangle_{12}=P_{21}\langle\exp[i\Phi_m]\rangle_{21}=-\frac{\varrho^m(1-\varrho^2)}{36\varrho^3} \times[(2\varrho-1)(1+3\varrho-\varrho^2) +(-1)^m(2\varrho+1)(1-3\varrho-\varrho^2)]\,, \quad (25b)$$

$$P_{22}\langle\exp[i\Phi_m]\rangle_{22}=\frac{\varrho^m(1-\varrho^2)^2}{36\varrho^3} \times[(2\varrho-1)+(-1)^m(2\varrho+1)]\,. \quad (25c)$$

Substitution of the above in equation (4) yields

$$\langle f_{m_3}f_{m'_3}\exp[i\Phi_m]\rangle/f^2=\frac{\varrho^m}{36\varrho^3} \times\{(2\varrho-1)[3\varrho-\sigma(2\varrho+1)(\varrho-2)]^2+(-1)^m(2\varrho+1) \times[3\varrho+\sigma(2\varrho-1)(\varrho+2)]^2\}\,. \quad m\geq 2\,. \quad (26)$$

The diffracted intensity

Expressions for the diffracted intensity can now be found by inserting the value of $\langle f_{m_3}f_{m'_3}\exp[i\Phi_m]\rangle$ from equations (12), (16), (18), (22), (26) in equation (1) and these are given below:

$$I(h_3, H-K=0 \text{ mod } 3) =\psi^2f^2\left[\sum_{m=-\infty}^{\infty}\left\{1+\frac{\sigma}{3}(4\varrho^2-1)\right\}^2\exp[i\pi mh_3]\right] +\psi^2f^2[(2\varrho^2+1)+(4\varrho^2-1)\cos\pi h_3] \times(1-\varrho^2)\cdot\frac{8\sigma^2}{9}\,; \quad (27a)$$

$$I(h_3, H-K \neq 0 \bmod 3)$$

$$= \psi^2 f^2 \left[-\frac{2\sigma(4\varrho^2-1)(1-\varrho^2)}{3\varrho^2} + \frac{2\sigma^2(2\varrho^2+1)(1-\varrho^2)}{9\varrho^2} - \frac{4\sigma^2(4\varrho^2-1)(1-\varrho^2)}{9\varrho^2} \cos \pi h_3 \right]$$

$$+ \psi^2 f^2 \cdot \frac{(2\varrho-1)\,[3\varrho-\sigma(2\varrho+1)(\varrho-2)]^2}{36\varrho^3} \times \frac{1-\varrho^2}{1-2\varrho\cos \pi h_3+\varrho^2}$$

$$+ \psi^2 f^2 \cdot \frac{(2\varrho+1)\,[3\varrho+\sigma(2\varrho-1)(\varrho+2)]^2}{36\varrho^3} \times \frac{1-\varrho^2}{1+2\varrho\cos \pi h_3+\varrho^2}. \tag{27b}$$

For $H-K=0$ mod 3, there is the usual sharp peak at $h_3=0$ mod 2. In addition, however, there is superimposed on this a broadened peak. The integrated intensities for the two are given respectively by

$$T_s=2\left[1+\frac{\sigma}{3}(4\varrho^2-1)\right]^2 \psi^2 f^2\,, \tag{28a}$$

$$T_b=\frac{32}{9}(1-\varrho^2)(1+2\varrho^2)\sigma^2\psi^2 f^2\,. \tag{28b}$$

For $H-K\neq 0$ mod 3, there are two broadened peaks at $h_3=0$ mod 2 and $h_3=1$ mod 2 respectively, which correspond to the second and third terms in equation (27*b*). The first term gives rise to a small broadened peak at $h_3=0$ mod 2. The integrated intensities T_0 and T_1 for reflexions at $h_3=0$ mod 2 and $h_3=1$ mod 2 respectively can be found by integrating equation (27*b*) within appropriate limits and are given by

$$T_0=\psi^2 f^2 \left[\frac{2\varrho-1}{2\varrho}+\frac{\sigma(4\varrho^2-1)(2\varrho-1)}{3\varrho}-\frac{\sigma^2}{18\pi\varrho^3} \times \{\pi(28\varrho^4-18\varrho^3-23\varrho^2+4)+16\varrho(4\varrho^2-1)(1-\varrho^2)\}\right], \tag{29a}$$

$$T_1=\psi^2 f^2 \left[\frac{2\varrho+1}{2\varrho}+\frac{\sigma(4\varrho^2-1)(2\varrho+1)}{3\varrho}+\frac{\sigma^2}{18\pi\varrho^3} \times \{\pi(28\varrho^4+18\varrho^3-23\varrho^2+4)+16\varrho(4\varrho^2-1)(1-\varrho^2)\}\right]. \tag{29b}$$

The ratio R of T_1 and T_0, to the first order in α, is given by

$$R=T_1/T_0=3\left[1+2\alpha\cdot\frac{1+2\sigma}{(1+\sigma)^2}\right]. \tag{30}$$

The integral breadths β_0 and β_1 for reflexions with $h_3=0$ mod 2 and $h_3=1$ mod 2 respectively are given by

$$\beta_0=\beta_1=\frac{3\alpha}{2} \tag{31}$$

to the first order in α and are thus unaffected by segregation.

The parameter σ, which depends upon segregation, can be found from the experimentally determined R, β_0 and β_1 by first evaluating α from equation (31) and then inserting this value in equation (30). This yields two values of σ, one positive and one negative. Physical considerations can now be used to pick out the actual value of σ from the two values thus found.

Normally σ may be expected to lie in the range

$$-0{\cdot}1<\sigma<+0{\cdot}1$$

and thus the maximum change in R would be less than a quarter per cent even for $\alpha=0{\cdot}1$. Since experimental errors in the measurement of R are usually much higher, the detection of segregation in a practical situation appears to be difficult. On the other hand, it is gratifying to know that α values are not affected by segregation of solute atoms to the faults.

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