parameters. While we cannot reject the proposal of Comes, Lambert & Guinier, the present analysis does show that it is in fact possible to determine the structure with reasonable accuracy when the correlation problem is avoided by the use of both X-ray and neutron diffraction data.

After this work was completed, the authors became aware of an unpublished refinement of a previous neutron diffraction analysis by Frazer (1962) with the following results:

$\Delta z_{\rm Ti} = 0{\cdot}014 \pm 0{\cdot}002$	$B_{33}({\rm Ba}) = 0{\cdot}42 \pm 0{\cdot}08$ Å^2
$\Delta z_{\rm O(1)} = 0{\cdot}0249 \pm 0{\cdot}0006$	$B_{33}({\rm Ti}) = 0{\cdot}45 \pm 0{\cdot}05$
$\Delta z_{\rm O(2)} = 0{\cdot}0156 \pm 0{\cdot}0007$	$B_{33}[{\rm O(1)}] = 0{\cdot}35 \pm 0{\cdot}04$
	$B_{33}[{\rm O(2)}] = 0{\cdot}47 \pm 0{\cdot}02$
	$B_{11}({\rm Ba}) = 0{\cdot}30 \pm 0{\cdot}02$
	$B_{11}({\rm Ti}) = 0{\cdot}56 \pm 0{\cdot}06$
	$B_{11}[{\rm O(1)}] = 0{\cdot}46 \pm 0{\cdot}02$
	$B_{11}[{\rm O(2)}] = 0{\cdot}55 \pm 0{\cdot}04$
	$B_{22}[{\rm O(2)}] = 0{\cdot}45 \pm 0{\cdot}02$

The position parameters of this refinement are in excellent agreement with our results, but the temperature parameters are not. Use of the above values with our X-ray and neutron data results in higher values of the reliability indices than those obtained with our position and temperature parameters.

We would like to thank Professor J. M. Cowley for his encouragement of the present study. We are grateful to Dr B. C. Frazer for permission to use the unpublished results of his refinement of neutron data and for useful discussions. We would also like to thank the staff of the solid state group of the AAEC and the Neutron Diffraction Group of the A.I.N.S.E. for their assistance, and Dr M. Mackay of the Chemistry Department of the University of Melbourne for making available the *ORFLS* program.

Financial support from the A.I.N.S.E. is gratefully acknowledged.

References

BUSING, W. R., MARTIN, K. O. & LEVY, H. A. (1962). *ORFLS*, Report ORNL-TM-305, Oak Ridge National Laboratory, Tennessee.
COMES, R., LAMBERT, M. & GUINIER, A. (1968). *C. R. Acad. Sci. Paris*, **266**, 959.
COOPER, M. J., ROUSE, K. D. & WILLIS, B. T. (1968). *Acta Cryst.* A**24**, 484.
COPPENS, P. (1968). *Acta Cryst.* B**24**, 1272.
CROMER, D. T. (1965). *Acta Cryst.* **18**, 17.
CROMER, D. T. & WABER, J. T. (1965). *Acta Cryst.* **18**, 105.
DANNER, H. R., FRAZER, B. C. & PEPINSKY, R. (1960). *Acta Cryst.* **13**, 1089.
EVANS, H. T. (1951). *Acta Cryst.* **4**, 377.
EVANS, H. T. (1951). *Acta Cryst.* **14**, 1019.
FRAZER, B. C. (1962). *J. Phys. Soc. Japan*, Suppl. B-II, 376.
FRAZER, B. C., DANNER, H. R. & PEPINSKY, R. (1955). *Phys. Rev.* **100**, 745.
GELLER, S. (1961). *Acta Cryst.* **14**, 1026.
HARADA, J. & HONJO, G. (1967). *J. Phys. Soc. Japan*, **22**, 45.
HARADA, J. & PEDERSEN, T. (1968). *J. Phys. Soc. Japan*, **25**, 1314.
International Tables for X-ray Crystallography (1959). Vol. II. Birmingham: Kynoch Press.
KITTEL, C. (1963). *Introduction to Solid State Physics*. New York: John Wiley.
RHODES, R. G. (1949). *Acta Cryst.* **2**, 417.
SHIRANE, G. & JONA, F. (1962). *Ferroelectric Crystals*. New York: Pergamon Press.
SHIRANE, G., JONA, F. & PEPINSKY, R. (1955). *Proc. Inst. Radio Engrs. N. Y.* **43**, 1738.
SHULL, C. G., WILKINSON, M. K. & MUELLER, M. H. (1960). *Phys. Rev.* **118**, 797.
ZACHARIASEN, W. H. (1963). *Acta Cryst.* **16**, 1139.

Acta Cryst. (1970). A**26**, 344

X-ray Diffraction from Hexagonal Close-Packed Crystals with Deformation Stacking Faults. II. Effect of Change in Layer Spacing at Faults

BY SHRIKANT LELE

Department of Metallurgy, Banaras Hindu University, Varanasi, India

(*Received* 31 *July* 1969)

The Christian–Gevers theory of X-ray diffraction from hexagonal close-packed crystals with deformation stacking faults is extended to include the effect of change in layer spacing at the faults. The results show that integral breadths as well as integrated intensities remain unaffected to a first approximation. The principal effect is to introduce peak shifts, the magnitude and direction of which depend on the reflexion.

Introduction

Diffraction effects due to the presence of deformation stacking faults in h.c.p. crystals are predicted under the following assumptions (Christian, 1954; Gevers, 1954; Lele, Anantharaman & Johnson, 1967):

(1) the crystal is infinite in size and is free from distortions;

(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 domains.

The effects of the simultaneous presence of stacking faults and strains in a finite crystal have been considered by Warren (1959), while the effects of changes in scattering power have been considered in part I (Lele, 1969).

Following Wagner, Tetelman & Otte (1962), a spacing fault may be defined as a displacement of a close-packed plane perpendicular to itself. A spacing fault thus changes the interlayer distance where it occurs. Such changes are unlikely to occur in close-packed metals because of the non-directional nature of the bonding. However, stacking faults produce localized regions of a different structure, which may give rise to a change in bond length and hence the lattice spacing. It thus appears that while spacing faults may not occur independently, they may occur in conjunction with stacking faults. Such a configuration is defined as a layer fault. Diffraction effects from spacing faults occurring in conjunction with deformation faults in face-centred cubic (f.c.c.) crystals have been described by Wagner, Tetelman & Otte (1962).

The present paper deals with the theory of X-ray diffraction from h.c.p. crystals with spacing and layer faults. The calculations have been made under assumptions (1), (2), (4) and (5) listed above.

The following considerations apply to layer faults only. Consider the sequence of close-packed (0002) layers in Fig. 1, where the faulted positions are denoted by F. A layer is designated hexagonal (h) if the layers adjacent to it are of the same type (*e.g.* B in the sequence ABA) and cubic (c) if they are of different types (*e.g.* B in the sequence ABC) (Jagodzinski, 1949). The spacings between layers of the type h and h, h and c, c and c may be expected to be different and are assumed to be $|\mathbf{A}_3|/2$, $(1+\delta/2)\,|\mathbf{A}_3|/2$, $(1+\delta)\,|\mathbf{A}_3|/2$ respectively. It may be noted that when several faults occur in succession, the f.c.c. structure is developed only at the boundaries of the set of faults, so that the spacings change only at these boundaries. Consequently, the total change in spacing in an m layer sequence is dependent not only on the total number of stacking faults but also on their arrangement in the crystal.

Formulation of the problem

We use the hexagonal axes $\mathbf{A}_1$, $\mathbf{A}_2$ and $\mathbf{A}_3$ ($|\mathbf{A}_3|$ being twice the interlayer spacing). The position vector of the atom m_1m_2 in the layer m_3 is given by

$$\mathbf{R}_m = m_1\mathbf{A}_1 + m_2\mathbf{A}_2 + \tfrac{1}{2}m_3\mathbf{A}_3 + \tfrac{1}{2}\mathbf{A}_3\delta p_{m_3} + \mathbf{f}q_{m_3}\,, \quad (1)$$

where $\frac{1}{2}\mathbf{A}_3\delta p_{m_3}$ and $\mathbf{f}q_{m_3}$ are respectively the displacements of layer m_3 perpendicular and parallel to its

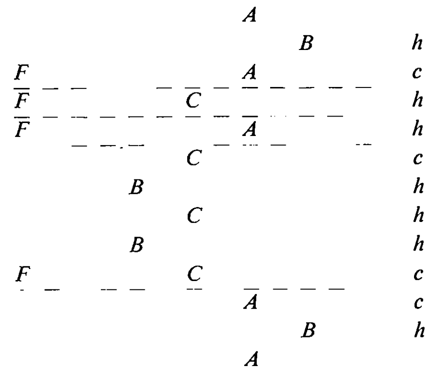

Fig. 1. Stacking sequences of (0002) planes. Faulted positions are denoted by F; the environment of the layers is indicated by h (hexagonal) or c (cubic).

own plane, and the stacking displacement vector

$$\mathbf{f} = \tfrac{1}{3}(\mathbf{A}_1 - \mathbf{A}_2)\,. \quad (2)$$

The diffracted intensity is given by

$$I(\mathbf{s}, \mathbf{s}_0) = \sum_m \sum_{m'} \exp\,[(2\pi i/\lambda)\,(\mathbf{s}-\mathbf{s}_0)\,.\,(\mathbf{R}_m - \mathbf{R}_{m'})]\,, \quad (3)$$

$\mathbf{s}_0$ and $\mathbf{s}$ being unit vectors in the direction of the incident and diffracted beams. In terms of the vectors $\mathbf{B}_1$, $\mathbf{B}_2$ and $\mathbf{B}_3$ (the reciprocals of $\mathbf{A}_1$, $\mathbf{A}_2$ and $\mathbf{A}_3$) and continuous parameters h_1, h_2 and h_3, we have

$$\frac{(\mathbf{s}-\mathbf{s}_0)}{\lambda} = h_1\mathbf{B}_1 + h_2\mathbf{B}_2 + h_3\mathbf{B}_3\,. \quad (4)$$

Substituting from equations (1), (2) and (4) in (3), we obtain

$$\begin{aligned} I(h_1h_2h_3) = \sum_m \sum_{m'} & \exp\,[2\pi i\{h_1(m_1-m_1') + h_2(m_2-m_2') \\ & + \tfrac{1}{2}h_3(m_3-m_3')\}] \\ & \times \exp\,[\pi i\{h_3\delta(p_{m_3}-p_{m_3'}) + (\tfrac{2}{3})\,(h_1-h_2) \\ & \times (q_{m_3}-q_{m_3'})\}]\,. \end{aligned} \quad (5)$$

Carrying out the summations over m_1, m_1', m_2 and m_2' and introducing

$$\left.\begin{aligned} m &= m_3 - m_3' \\ p_m &= p_{m_3} - p_{m_3'} \\ q_m &= q_{m_3} - q_{m_3'} \end{aligned}\right\} \quad (6)$$

we get

$$I(h_3) = \psi^2 \sum_{m_3} \sum_m \exp\,[\pi i m h_3] \exp\,[i\varphi_m]\,, \quad (7)$$

where ψ^2 is a function of h_1 and h_2, which vanishes except when $h_1 = H$ and $h_2 = K$ and

$$\varphi_m = \pi h_3 \delta p_m + \frac{2\pi}{3}\,(H-K) q_m\,. \quad (8)$$

Since p_m and q_m and hence φ_m are stochastic variables taking different values for different m_3, we may replace $\exp[i\varphi_m]$ by its average and drop the summation over m_3. Thus

$$I(h_3)=\psi^2\sum_m \exp[\pi imh_3]\langle\exp[i\varphi_m]\rangle\,. \qquad (9)$$

Two types of planes can be distinguished in the h.c.p. structure. A plane is of 'A' type if, in the absence of a fault, $q_1=+1$; it is of 'B' type if $q_1=-1$. The phase differences φ_m^A and φ_m^B in a sequence of m planes starting with A and B type planes respectively are given by

$$\varphi^A_{m,p,k_1,k_2}=\pi h_3\delta p + \frac{2\pi}{3}(H-K)\left[\frac{1-(-1)^m}{2}+2(k_1-k_2)\right]; \qquad (10a)$$

$$\varphi^B_{m,p,k_1,k_2}=\pi h_3\delta p - \frac{2\pi}{3}(H-K)\left[\frac{1-(-1)^m}{2}+2(k_1-k_2)\right]; \qquad (10b)$$

where k_1 and k_2 are the numbers of faults on the even – and odd – numbered planes respectively and p is a particular value of p_m(compatible with the presence of the above number of faults in the case of layer faults). For spacing faults only, $k_1=k_2=0$ and p becomes simply the number of spacing faults.

Spacing faults

The probability of obtaining a phase difference $\varphi^A_{m,p}$ (or $\varphi^B_{m,p}$) is simply the product of the probability $P(A)$ [or $P(B)$] of having an A (or B) type plane at the origin and the probability $P(m,p)$ of obtaining p spacing faults in an m plane sequence. Since

$$P(A)=P(B)=\tfrac{1}{2}\,,$$

we may write

$$\langle\exp[i\varphi_m]\rangle = \tfrac{1}{2}\sum_p P(m,p)\{\exp[i\varphi^A_{m,p}]+\exp[i\varphi^B_{m,p}]\}. \qquad (11)$$

To evaluate $P(m,p)$, consider an m plane sequence with p spacing faults. This may be obtained from $(m-1)$ plane sequences with $(p-1)$ and p spacing faults respectively by adding the mth plane with and without a spacing fault. Thus

$$P(m,p)=\alpha P(m-1,p-1)+(1-\alpha)P(m-1,p)\,, \qquad (12)$$

where α is the probability of the occurrence of a fault. The solution of this difference equation is

$$P(m,p)=\frac{m!}{p!(m-p)!}\,\alpha^p(1-\alpha)^{m-p}\,. \qquad (13)$$

Considering the cases $H-K=0$ mod 3 and $H-K\neq 0$ mod 3 separately and substituting from equations (10) and (13) in (11), we get, after simplification,

$$\langle\exp[i\varphi_m]\rangle=\exp[\pi imh_3\alpha\delta] \quad \text{for} \quad H-K=0 \text{ mod } 3,\ \delta\ll 1\,, \qquad (14a)$$

$$\langle\exp[i\varphi_m]\rangle=\tfrac{1}{4}[1+3(-1)^m]\exp[\pi imh_3\alpha\delta] \quad \text{for} \quad H-K\neq 0 \text{ mod } 3,\ \delta\ll 1\,. \qquad (14b)$$

The above expressions are approximations valid only for small values of δ. Substitution in equation (9) gives for the diffracted intensity

$$I(h_3)=\psi^2\sum_m \exp[\pi imh_3\alpha\delta]\exp[\pi imh_3] = \psi^2\sum_m \cos\left[2\pi m\left\{\frac{h_3(1+\alpha\delta)-L}{2}+\frac{L}{2}\right\}\right]$$
$$\text{for} \quad H-K=0 \text{ mod } 3,\ \delta\ll 1\,, \qquad (15a)$$

$$I(h_3)=\frac{\psi^2}{4}\sum_m[1+3(-1)^m]\exp[\pi imh_3\alpha\delta]\exp[\pi imh_3] = \frac{\psi^2}{4}\sum_m\cos\left[2\pi m\left\{\frac{h_3(1+\alpha\delta)-L}{2}+\frac{L}{2}\right\}\right] + \frac{3\psi^2}{4}\sum_m\cos\left[2\pi m\left\{\frac{h_3(1+\alpha\delta)-L}{2}+\frac{L+1}{2}\right\}\right]$$
$$\text{for} \quad H-K\neq 0 \text{ mod } 3,\ \delta\ll 1\,. \qquad (15b)$$

For $H-K=0$ mod 3, the intensity has a sharp symmetrical peak at $h_3=L(1+\alpha\delta)^{-1}$ if L is even. There is thus a peak shift of $-L\alpha\delta$. For $H-K\neq 0$ mod 3, the first term in equation (15b) gives a sharp symmetrical peak at $h_3=L(1+\alpha\delta)^{-1}$ if L is even and the second gives a sharp symmetrical peak at $h_3=L(1+\alpha\delta)^{-1}$ if L is odd. Again the peak shift is $-L\alpha\delta$. The peak shift in terms of 2θ is given by

$$\Delta(2\theta)^\circ=-\frac{360}{\pi}\cdot\frac{L^2d^2}{c^2}\cdot(\tan\theta)\,.\,\alpha\delta,\quad \delta\ll 1 \qquad (16)$$

for all reflexions. It may be noted that the peak shifts are equivalent to a change of the c parameter to $c(1+\alpha\delta)$.

Layer faults

An equation analogous to equation (11) for the case of spacing faults may be written as follows:

$$\langle\exp[i\varphi_m]\rangle=\tfrac{1}{2}\sum_p\sum_{k_1}\sum_{k_2}P(m,p,k_1,k_2)\{\exp[i\varphi^A_{m,p,k_1,k_2}]+\exp[i\varphi^B_{m,p,k_1,k_2}]\}\,, \qquad (17)$$

where $P(m,p,k_1,k_2)$ is the probability of having k_1 and k_2 faults on even- and odd-numbered planes respectively, distributed so that they give rise to an additional shift of p in a direction perpendicular to the stacking plane. To evaluate $P(m,p,k_1,k_2)$, consider an m plane sequence. Now add the $(m+1)$th layer. This may be done without the introduction of a fault with probability $(1-\alpha)$ or with the introduction of a fault with probability α. The mth plane may be of hexagonal or cubic type depending on the relative positions of the $(m-1)$th and $(m+1)$th planes with respect to it. Thus there are four possibilities:

(1) the mth plane is hexagonal and the $(m+1)$th plane is added without a fault;
(2) the mth plane is hexagonal and the $(m+1)$th plane is added with the introduction of a fault;

(3) the mth plane is cubic and the $(m+1)$th plane is added without a fault;
(4) the mth plane is cubic and the $(m+1)$th plane is added with the introduction of a fault.

Let the probabilities for the above four possibilities be $P^{hu}(m,p,k_1,k_2)$, $P^{hf}(m,p,k_1,k_2)$, $P^{cu}(m,p,k_1,k_2)$ and $P^{cf}(m,p,k_1,k_2)$ respectively (the letters h, c, u and f in the superscripts stand for hexagonal, cubic, unfaulted and faulted respectively). It is obvious that

$$P(m,p,k_1,k_2)=P^{hu}(m,p,k_1,k_2)+P^{hf}(m,p,k_1,k_2)+P^{cu}(m,p,k_1,k_2)+P^{cf}(m,p,k_1,k_2)\,. \quad (18)$$

Remembering that additional displacements $(\delta/2)$ $(|\mathbf{A}_3|/2)$ and (δ) $(|\mathbf{A}_3|/2)$ perpendicular to the close-packed planes occur between pairs of planes of the type ch and cc respectively, and further that faults occurring on even- and odd-numbered planes are counted in k_1 and k_2 respectively, the following recurrence relations can be derived:

$$P^{hu}(2m+1,p,k_1,k_2)=(1-\alpha)\,[P^{hu}(2m,p,k_1,k_2)+P^{cu}(2m,p-\tfrac{1}{2},k_1,k_2)]\,,\quad m\ge 0\,,\quad (19a)$$

$$P^{hf}(2m+1,p,k_1,k_2)=\alpha[P^{hf}(2m,p,k_1,k_2-1)+P^{cf}(2m,p-\tfrac{1}{2},k_1,k_2-1)]\,,\quad m\ge 0\,,\quad (19b)$$

$$P^{cu}(2m+1,p,k_1,k_2)=(1-\alpha)\,[P^{hf}(2m,p-\tfrac{1}{2},k_1,k_2-1)+P^{cf}(2m,p-1,k_1,k_2-1)]\,,\quad m\ge 0\,,\quad (19c)$$

$$P^{cf}(2m+1,p,k_1,k_2)=\alpha[P^{hu}(2m,p-\tfrac{1}{2},k_1,k_2)+P^{cu}(2m,p-1,k_1,k_2)]\,,\quad m\ge 0\,,\quad (19d)$$

$$P^{hu}(2m,p,k_1,k_2)=(1-\alpha)\,[P^{hu}(2m-1,p,k_1,k_2)+P^{cu}(2m-1,p-\tfrac{1}{2},k_1,k_2)]\,,\quad m\ge 1\,,\quad (19e)$$

$$P^{hf}(2m,p,k_1,k_2)=\alpha[P^{hf}(2m-1,p,k_1-1,k_2)+P^{cf}(2m-1,p-\tfrac{1}{2},k_1-1,k_2)]\,,\quad m\ge 1\,,\quad (19f)$$

$$P^{cu}(2m,p,k_1,k_2)=(1-\alpha)\,[P^{hf}(2m-1,p-\tfrac{1}{2},k_1-1,k_2)+P^{cf}(2m-1,p-1,k_1-1,k_2)]\,,\quad m\ge 1\,,\quad (19g)$$

$$P^{cf}(2m,p,k_1,k_2)=\alpha[P^{hu}(2m-1,p-\tfrac{1}{2},k_1,k_2)+P^{cu}(2m-1,p-1,k_1,k_2)]\,,\quad m\ge 1\,.\quad (19h)$$

Solving equations (19a), (19b), (19c) and (19f) for $P^{cu}(2m,p-\frac{1}{2},k_1,k_2)$, $P^{cf}(2m,p-\frac{1}{2},k_1,k_2-1)$, $P^{cu}(2m-1,p-\frac{1}{2},k_1,k_2)$ and $P^{cf}(2m-1,p-\frac{1}{2},k_1-1,k_2)$ respectively and substituting these values in equations (19c), (19d), (19g) and (19h), we obtain

$$\alpha^2P^{hu}(2m+1,p-\tfrac{1}{2},k_1,k_2)=(1-\alpha)P^{hf}(2m+2,p+\tfrac{1}{2},k_1+1,k_2)-\alpha(1-\alpha)P^{hf}(2m+1,p+\tfrac{1}{2},k_1,k_2)\,,\quad m\ge 0\,,\quad (20a)$$

$$(1-\alpha)^2P^{hf}(2m+1,p-\tfrac{1}{2},k_1,k_2)=\alpha P^{hu}(2m+2,p+\tfrac{1}{2},k_1,k_2)-\alpha(1-\alpha)P^{hu}(2m+1,p+\tfrac{1}{2},k_1,k_2)\,,\quad m\ge 0\,,\quad (20b)$$

$$\alpha^2P^{hu}(2m,p-\tfrac{1}{2},k_1,k_2)=(1-\alpha)P^{hf}(2m+1,p+\tfrac{1}{2},k_1,k_2+1)-\alpha(1-\alpha)P^{hf}(2m,p+\tfrac{1}{2},k_1,k_2)\,,\quad m\ge 1\,,\quad (20c)$$

$$(1-\alpha)^2P^{hf}(2m,p-\tfrac{1}{2},k_1,k_2)=\alpha P^{hu}(2m+1,p+\tfrac{1}{2},k_1,k_2)-\alpha(1-\alpha)P^{hu}(2m,p+\tfrac{1}{2},k_1,k_2)\,,\quad m\ge 1\,.\quad (20d)$$

Substituting from equations (20b) and (20d) for $P^{hf}(2m+1,p-\frac{1}{2},k_1,k_2)$ and $P^{hf}(2m,p-\frac{1}{2},k_1,k_2)$ respectively in equations (20a) and (20c), we have, after rearrangement,

$$\begin{aligned}(1-\alpha)P^{hu}(2m+2,p+\tfrac{3}{2},k_1+1,k_2)+\alpha P^{hu}(2m+2,p+\tfrac{3}{2},k_1,k_2)={}&P^{hu}(2m+3,p+\tfrac{3}{2},k_1+1,k_2)\\&+\alpha(1-\alpha)\,[P^{hu}(2m+1,p+\tfrac{3}{2},k_1,k_2)\\&-P^{hu}(2m+1,p-\tfrac{1}{2},k_1,k_2)]\,,\quad m\ge 0\,,\quad (21a)\end{aligned}$$

$$\begin{aligned}(1-\alpha)P^{hu}(2m+1,p+\tfrac{3}{2},k_1,k_2+1)+\alpha P^{hu}(2m+1,p+\tfrac{3}{2},k_1,k_2)={}&P^{hu}(2m+2,p+\tfrac{3}{2},k_1,k_2+1)\\&+\alpha(1-\alpha)\,[P^{hu}(2m,p+\tfrac{3}{2},k_1,k_2)\\&-P^{hu}(2m,p-\tfrac{1}{2},k_1,k_2)]\,,\quad m\ge 1\,.\quad (21b)\end{aligned}$$

Inserting (k_1-1) in place of k_1 in equation (21b), we get

$$\begin{aligned}(1-\alpha)P^{hu}(2m+1,p+\tfrac{3}{2},k_1-1,k_2+1)+\alpha P^{hu}(2m+1,p+\tfrac{3}{2},k_1-1,k_2)={}&P^{hu}(2m+2,p+\tfrac{3}{2},k_1-1,k_2+1)\\&+\alpha(1-\alpha)\,[P^{hu}(2m,p+\tfrac{3}{2},k_1-1,k_2)\\&-P^{hu}(2m,p-\tfrac{1}{2},k_1-1,k_2)]\,,\quad m\ge 1\,.\quad (21c)\end{aligned}$$

Multiplying equations (21b) and (21c) by $(1-\alpha)$ and α respectively, adding them, substituting from equation (21a) and simplifying, we get

$$\begin{aligned}P^{hu}(2m+3,p+\tfrac{3}{2},k_1,k_2+1)={}&(1-\alpha)^2P^{hu}(2m+1,p+\tfrac{3}{2},k_1,k_2+1)\\&+\alpha^2P^{hu}(2m+1,p+\tfrac{3}{2},k_1-1,k_2)\\&+\alpha(1-\alpha)[P^{hu}(2m+1,p-\tfrac{1}{2},k_1-1,k_2+1)\\&+P^{hu}(2m+1,p-\tfrac{1}{2},k_1,k_2)]\\&-\alpha^2(1-\alpha)^2[P^{hu}(2m-1,p+\tfrac{3}{2},k_1-1,k_2)\\&-2P^{hu}(2m-1,p-\tfrac{1}{2},k_1-1,k_2)\\&+P^{hu}(2m-1,p-\tfrac{5}{2},k_1-1,k_2)]\,,\quad m\ge 1\,.\quad (22)\end{aligned}$$

Similar expressions can be found for $P^{hf}(2m+1,p,k_1,k_2)$ *etc.* and utilizing equation (18), we obtain

$$\begin{aligned}P(m,p,k_1,k_2)={}&(1-\alpha)^2P(m-2,p,k_1,k_2)\\&+\alpha^2P(m-2,p,k_1-1,k_2-1)\\&+\alpha(1-\alpha)\,[P(m-2,p-2,k_1,k_2-1)\\&+P(m-2,p-2,k_1-1,k_2)]\\&-\alpha^2(1-\alpha)^2[P(m-4,p,k_1-1,k_2-1)\\&-2P(m-4,p-2,k_1-1,k_2-1)\\&+P(m-4,p-4,k_1-1,k_2-1)]\,,\quad m\ge 5\,.\quad (23)\end{aligned}$$

Instead of solving this difference equation, we will solve a simpler difference equation in $\langle \exp [i\varphi_m] \rangle$, which can be obtained by substitution from equations (10) and (23) in equation (17).

(i) $H-K=0 \bmod 3$

From equation (10), φ_m is independent of k_1 and k_2 and therefore the probability $P(m, p)$ should be used in equation (17), where $P(m, p)$ is the probability of obtaining an additional phase shift $\pi h_3 \delta p$ in an m plane sequence irrespective of the number of faults. A little consideration shows that

$$P(m, p) = \sum_{k_1} \sum_{k_2} P(m, p, k_1, k_2) . \quad (24)$$

Substituting from equation (23) in the above, we get

$$\begin{aligned} P(m, p) &= (1-2\gamma)P(m-2, p) \\ &+ 2\gamma P(m-2, p-2) + 2\gamma^2 P(m-4, p-2) \\ &- \gamma^2 [P(m-4, p) + P(m-4, p-4)] , \quad m \geq 5 , \end{aligned} \quad (25)$$

where $\gamma = \alpha(1-\alpha) \simeq \alpha$ for small values of α. From equations (10), (17) and (25), we get

$$\begin{aligned} \langle \exp [i\varphi_m] \rangle &= \{(1-2\gamma) + 2\gamma \exp [2\pi i h_3 \delta]\} \langle \exp [i\varphi_{m-2}] \rangle \\ &- \gamma^2 \{1 - \exp [2\pi i h_3 \delta]\}^2 \langle \exp [i\varphi_{m-4}] \rangle , \quad m \geq 5 . \end{aligned} \quad (26)$$

Letting

$$\langle \exp [i\varphi_m] \rangle = C x^m , \quad m \geq 1 , \quad (27)$$

we obtain from equation (26)

$$\begin{aligned} x^4 - \{(1-2\gamma) + 2\gamma \exp [2\pi i h_3 \delta]\} x^2 \\ + \gamma^2 \{1 - \exp [2\pi i h_3 \delta]\}^2 = 0 , \end{aligned} \quad (28)$$

the solutions of which are

$$x = \pm \tfrac{1}{2} [1 \pm \{1 - 4\gamma + 4\gamma \exp [2\pi i h_3 \delta]\}^{1/2}] . \quad (29)$$

Utilizing the initial conditions

$$\begin{aligned} \langle \exp [i\varphi_1] \rangle &= 1 - 3\gamma + 2\gamma \exp [\pi i h_3 \delta/2] \\ &+ \gamma \exp [\pi i h_3 \delta] , \end{aligned} \quad (30a)$$

$$\begin{aligned} \langle \exp [i\varphi_2] \rangle &= 1 - 4\gamma + 2\gamma^2 + 2\gamma(1-2\gamma) \exp [\pi i h_3 \delta/2] \\ &+ 4\gamma^2 \exp [\pi i h_3 \delta] + 2\gamma(1-2\gamma) \exp [3\pi i h_3 \delta/2] \\ &+ 2\gamma^2 \exp [2\pi i h_3 \delta] , \end{aligned} \quad (30b)$$

we get from equations (26), (27) and (29)

$$\langle \exp [i\varphi_m] \rangle = \exp [2\pi i m h_3 \gamma \delta] \quad \text{for} \quad H-K=0 \bmod 3 , \quad \delta \ll 1 \quad (31)$$

for small δ. Substitution in equation (9) gives for the intensity

$$\begin{aligned} I(h_3) &= \psi^2 \sum_m \exp [2\pi i m h_3 \gamma \delta] \exp [\pi i m h_3] \\ &= \psi^2 \sum_m \cos \left[2\pi m \left\{ \frac{h_3(1+2\gamma\delta) - L}{2} + \frac{L}{2} \right\} \right] \end{aligned}$$

$$\text{for} \quad H-K=0 \bmod 3 , \quad \delta \ll 1 . \quad (32)$$

This expression represents a sharp symmetrical peak at $h_3 = L(1+2\gamma\delta)^{-1}$ for L even. There is a peak shift which in terms of 2θ is given by

$$\Delta(2\theta)^\circ = -\frac{720}{\pi} \cdot \frac{L^2 d^2}{c^2} \cdot (\tan \theta) \cdot \gamma\delta$$
$$\text{for} \quad H-K=0 \bmod 3 , \quad \delta \ll 1 . \quad (33)$$

(ii) $H-K \neq 0 \bmod 3$

Substituting from equations (10) and (23) in (17), we get

$$\begin{aligned} \langle \exp [i\varphi_m] \rangle &= \{(1-2\gamma) - \gamma \exp [2\pi i h_3 \delta]\} \langle \exp [i\varphi_{m-2}] \rangle \\ &- \gamma^2 \{1 - \exp [2\pi i h_3 \delta]\}^2 \langle \exp [i\varphi_{m-4}] \rangle , \\ & \qquad m \geq 5 . \end{aligned} \quad (34)$$

Let the solution of this equation be of the form

$$\langle \exp [i\varphi_m] \rangle = C y^m , \quad m \geq 1 , \quad (35)$$

so that

$$\begin{aligned} y = \pm \frac{1}{\sqrt{2}} & [1 - 2\gamma - \gamma \exp [2\pi i h_3 \delta] \\ & \pm \{(1 - 3\gamma \exp [2\pi i h_3 \delta]) \\ & \times (1 - 4\gamma + \gamma \exp [2\pi i h_3 \delta])\}^{1/2}]^{1/2} . \end{aligned} \quad (36)$$

The solution of equation (34) can be obtained by using the initial conditions:

$$\begin{aligned} \langle \exp [i\varphi_1] \rangle &= -\tfrac{1}{2} \{1 - 3\gamma + 2\gamma \exp [\pi i h_3 \delta/2] \\ &+ \gamma \exp [\pi i h_3 \delta]\} , \end{aligned} \quad (37a)$$

$$\begin{aligned} \langle \exp [i\varphi_2] \rangle &= 1 - 4\gamma + 2\gamma^2 + 2\gamma(1-2\gamma) \exp [\pi i h_3 \delta/2] \\ &+ \gamma^2 \exp [\pi i h_3 \delta] \\ &- \gamma(1-2\gamma) \exp [3\pi i h_3 \delta/2] - \gamma^2 \exp [2\pi i h_3 \delta] , \end{aligned} \quad (37b)$$

in conjunction with equations (35) and (36). Thus

$$\langle \exp [i\varphi_m] \rangle = \left[\frac{2\varrho - 1}{4\varrho} + (-1)^m \cdot \frac{2\varrho + 1}{4\varrho} \right] \varrho^{|m|} \times \exp [-\pi i |m| h_3 \gamma \delta]$$
$$\text{for} \quad H-K \neq 0 \bmod 3 , \quad \delta \ll 1 , \quad (38)$$

where

$$\varrho = (1 - 3\gamma)^{1/2} . \quad (39)$$

Substitution in equation (9) gives for the intensity

$$\begin{aligned} I(h_3) &= \psi^2 \cdot \frac{2\varrho - 1}{4\varrho} \sum_m \varrho^{|m|} \exp [\pi i |m| h_3 (1 - \gamma\delta)] \\ &+ \psi^2 \cdot \frac{2\varrho + 1}{4\varrho} \sum_m (-\varrho)^{|m|} \exp [\pi i |m| h_3 (1 - \gamma\delta)] \end{aligned}$$
$$\text{for} \quad H-K \neq 0 \bmod 3 , \quad \delta \ll 1 . \quad (40)$$

Summing the geometric series in equation (40), we obtain

$$I(h_3)=\psi^2 \cdot \frac{2\varrho-1}{4\varrho} \cdot \frac{1-\varrho^2}{1-2\varrho \cos [\pi h_3(1-\gamma\delta)]+\varrho^2}$$
$$+\psi^2 \cdot \frac{2\varrho+1}{4\varrho} \cdot \frac{1-\varrho^2}{1+2\varrho \cos [\pi h_3(1-\gamma\delta)]+\varrho^2}$$
$$\text{for} \quad H-K\neq 0 \bmod 3\,, \quad \delta \ll 1\,. \quad (41)$$

The first term on the right hand side of equation (41) represents a symmetrically broadened peak at $h_3=L(1-\gamma\delta)^{-1}$ for L even, while the second represents a symmetrically broadened peak at $h_3=(1-\gamma\delta)^{-1}$ for L odd. There is thus a peak shift which in 2θ coordinates is given by

$$\Delta(2\theta)^\circ = + \frac{360}{\pi} \cdot \frac{L^2d^2}{c^2} \cdot (\tan\theta) \cdot \gamma\delta$$
$$\text{for} \quad H-K\neq 0 \bmod 3\,, \quad \delta \ll 1\,. \quad (42)$$

Conclusions

To summarize the results, we find that spacing faults give rise to peak shifts for all reflexions which are equivalent to a change of the c parameter to $c(1+\alpha\delta)$. There are no changes in the integrated intensity and the reflexions remain sharp and symmetrical. The results for layer faults are slightly complicated in that reflexions with $H-K=0$ mod 3 are shifted twice as much as those with $H-K\neq 0$ mod 3 and in the opposite direction. Again, the integrated intensity or the broadening is not affected by layer faults.

An estimate of $\alpha\delta$ can be obtained from measurements of peak shifts for spacing as well as layer faults. In the case of layer faults the parameter α can be estimated independently from measurements of the integral breadths. Inserting this value in $\alpha\delta$, one can obtain δ.

Finally, we note that since deformation stacking faults give rise to changes in integrated intensity and to peak broadening but not to peak shifts, estimates of α are not affected by changes in layer spacing at the faults.

The author is grateful to Dr T. R. Anantharaman, Professor and Head, Department of Metallurgy, Banaras Hindu University, for encouragement and to the University Grants Commission, New Delhi, for the award of a Senior Research Fellowship.

References

CHRISTIAN, J. W. (1954). *Acta Cryst.* **7**, 415.
GEVERS, R. (1954). *Acta Cryst.* **7**, 337.
JAGODZINSKI, H. (1949). *Acta Cryst.* **2**, 201.
LELE, S. (1969). *Acta Cryst.* A**25**, 351.
LELE, S., ANANTHARAMAN, T. R. & JOHNSON, C. A. (1967). *Phys. Stat. Sol.* **20**, 59.
WAGNER, C. N. J., TETELMAN, A. S. & OTTE, H. M. (1962). *J. Appl. Phys.* **33**, 3080.
WARREN, B. E. (1959). *Progr. Met. Phys.* **8**, 147.

Acta Cryst. (1970). A**26**, 349

Contrast Reversal of Kikuchi Lines with Specimen Thickness

BY YASUO NAKAI
Department of Physics, Nagoya University, Nagoya, Japan

(*Received* 29 *May* 1969 *and in revised form* 11 *August* 1969)

In normal Kikuchi patterns a defect line and an excess line pass through the incident spot and a diffracted spot respectively, when the Bragg condition is satisfied. By means of selected area diffraction at 80 kV accelerating voltage, Kikuchi patterns were recorded from various thicknesses of a silicon crystal. Normal contrast was obtained from regions where the thickness was $(n+\frac{1}{2})l$, where l is the extinction distance and n is an integer, while the contrast was reversed for those regions where the thickness was nl. This result, can be explained by a theory of inelastic scattering; it is contrary to that obtained by Thomas & Bell (*Proc. Fourth European Regional Conf. Electron Microscopy*, Rome (1968), 283) where normal contrast was obtained for nl and reversed contrast for $(n+\frac{1}{2})l$.

1. Introduction

Electron diffraction patterns from fairly thick specimens (several thousand Ångstrom) consist of Bragg spots and Kikuchi patterns. Kikuchi (1928) interpreted Kikuchi lines as being the interference pattern from Bragg reflexion of inelastically scattered electrons, and the main features of their geometry and contrast (excess or defect) were explained by this simple theory.

Secondary maxima in the Kikuchi lines similar to those observed in the case of diffraction spots were observed by Uyeda, Fukano & Ichinokawa (1954) in diffraction patterns from a thin film of molybdenite. Kainuma's (1955) theory of Kikuchi lines explains