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X-ray Diffraction by Close-Packed Crystals with 'Growth-' and 'Deformation or Transformation Stacking Faults' Assuming an '*n*-Layer Influence'

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The general theory is developed of the X-ray diffraction effects exhibited by close-packed crystals containing both 'growth-' and 'deformation or transformation stacking faults'.

A general '*n*-layer influence' is postulated for the distribution of the 'faults' of the first and also for those of the second type.

This means that: (1) the probability α_i for a layer to be k-arranged in the original pattern of close-packed layers, depends on the arrangement of its n predecessors; (2) the probability β_j for a layer to be a 'deformation or transformation stacking fault' depends on the arrangement of 'correct' and 'fault' layers in the sequence of its n predecessors. A general expression can then be derived for the reciprocal-lattice X-ray intensity distribution as a function of the 2^{n-2} parameters α_i and the 2^n parameters β_j.

The formulae are given for the special cases (*a*) an irregular pattern in which the 'faults of the second type' are randomly distributed, or are not present; (*b*) an irregular pattern obtained by introducing 'faults of the second type' into an hexagonal or cubic close-packed pattern with randomly distributed 'faults of the first type'; (*c*) an irregular pattern obtained by introducing 'faults of the second type' into a regular cubic close-packed pattern. For the last case we give the general expression for the X-ray intensity, as it differs from that which covers all the other cases.

1. Introduction

1. It has been proved (Jagodzinski, 1949) that the X-ray intensity diffracted by close-packed crystals with 'stacking faults' is

$$I = |F|^2 \frac{\sin^2 \frac{1}{2}N_1A_1}{\sin^2 \frac{1}{2}A_1} \cdot \frac{\sin^2 \frac{1}{2}N_2A_2}{\sin^2 \frac{1}{2}A_2} \times \left[\frac{1+2Q}{3} \cdot \frac{\sin^2 \frac{1}{2}N_3A_3}{\sin^2 \frac{1}{2}A_3} + (1-Q) \sum_r \frac{C_r N_3(1-x_r^2)}{1-2x_r \cos A_3 + x_r^2}\right], \quad (1)$$

where x_r are the roots of a characteristic equation, and where the C_r's are the solution of the system

$$\sum_r C_r x_r^m = P_m - \tfrac{1}{3}. \quad (2)$$

2. In this article we shall calculate the characteristic equation in the general case of an '*n*-layer influence' for both types of 'faults' (Gevers, 1954*a*). We consider a close-packed crystal with irregularly stacked layers, grown so that an 'n-layer influence' exists. As described in a previous article (Gevers, 1954*b*), any layer can be the last of a succession of n layers, which may be arranged in $2^{n-2} = 4l$ ways a_i. These can be numbered so that we have:

$$a_{2i-\lambda} \quad (i=1,\ldots,2l)(\lambda=0,1) \longrightarrow a_i \text{ prob. } (1-\alpha_{2i-\lambda}), \quad (3a)$$

$$a_{2i-\lambda} \quad (i=1,\ldots,2l)(\lambda=0,1) \longrightarrow a_{i+2l} \text{ prob. } \alpha_{2i-\lambda}, \quad (3b)$$

where the $\alpha_{2i-\lambda}$'s are the $4l$ transition probabilities (Gevers, 1954*b*, formulae (3) and (5)).

Suppose now that 'deformation or transformation stacking faults' (Gevers, 1954*a*) are introduced in this irregular pattern. We shall consider here the general case that there is a general '*n*-layer influence' for the distribution of these 'faults'. This means: n layers can be arranged, in sequences of 'correct' (C) or 'fault' (F) layers, in $2^n = 16l$ ways a^j. For a layer which is the last of a series of n layers in an a^j arrangement (in C- and F-layers) the probability β_j of its being followed by a 'deformation or transformation stacking fault' will depend on that arrangement a^j. The $16l$ ways a^j can be numbered in a manner completely analogous to the one we used to number the a_i-ways. Consequently we have:

$$a^{2j-\mu} \longrightarrow a^j \text{ prob. } (1-\beta_{2j-\mu}), \quad (4a)$$

$$a^{2j-\mu} \quad (j=1,\ldots,8l)(\mu=0,1) \longrightarrow a^{j+8l} \text{ prob. } \beta_{2j-\mu}. \quad (4b)$$

On introducing 'faults of the second type' into the pattern already disturbed by 'faults' of the first type, we obtain a succession of close-packed layers in which a given layer can be the last of the sequence of n-layers in one of the $8l \times 4l = 32l^2$ arrangements $a_i^j \left(\substack{j=1,\ldots,16l \\ i=1,\ldots,4l}\right)$.

We shall say that n successive layers in the irregular stacking, resulting from the presence of 'faults' of both types, are in an a_i^j-arrangement, if (1) these n-layers were a_i-arranged in the pattern existing before the introduction of the 'faults' of the second type; (2) these n-layers form, after that introduction, an a^j-sequence of C and F layers.

If (3) and (4) are taken into account, the succession of the close-packed layers is given by the rule:

$$a_{2i-\lambda}^{2j-\mu}\ (i=1,\ldots,2l)(\lambda=0,1).\ (j=1,\ldots,8l)(\mu=0,1).$$

$$\longrightarrow a_i^j \quad \text{prob. } (1-\alpha_{2i-\lambda})(1-\beta_{2j-\mu}), \tag{5a}$$

$$\longrightarrow a_i^{j+8l} \text{ prob. } (1-\alpha_{2i-\lambda})\beta_{2j-\mu}, \tag{5b}$$

$$\longrightarrow a_{i+2l}^{j} \text{ prob. } \alpha_{2i-\lambda}(1-\beta_{2j-\mu}), \tag{5c}$$

$$\longrightarrow a_{i+2l}^{j+8l} \text{ prob. } \alpha_{2i-\lambda}\beta_{2j-\mu}. \tag{5d}$$

3. Let W_i^j be the probability that a given layer is in an a_i^j-arrangement with its $(n-1)$ predecessors, and P_m the probability that two layers, m layers apart, are in the relationship $A(B,C)\ldots A(B,C)$, while $p_m\binom{j}{i}$ will be the partial probability that the last of these two layers (layer 0 and layer m) is in the arrangement a_i^j. Then we have

$$\sum_{i=1}^{4l}\sum_{j=1}^{16l} W_i^j = 1 \tag{6a}$$

and

$$P_m = \sum_{i=1}^{4l}\sum_{j=1}^{16l} p_m\binom{j}{i}. \tag{6b}$$

4. With the aid of (5) we obtain:

$$W_i^j = \sum_{\lambda=0}^{1}\sum_{\mu=0}^{1} W_{2i-\lambda}^{2j-\mu}(1-\alpha_{2i-\lambda})(1-\beta_{2j-\mu}), \tag{7a}$$

$$W_i^{j+8l} = \sum_{\lambda=0}^{1}\sum_{\mu=0}^{1} W_{2i-\lambda}^{2j-\mu}(1-\alpha_{2i-\lambda})\beta_{2j-\mu}, \tag{7b}$$

$$W_{i+2l}^{j} = \sum_{\lambda=0}^{1}\sum_{\mu=0}^{1} W_{2i-\lambda}^{2j-\mu}\alpha_{2i-\lambda}(1-\beta_{2j-\mu}), \tag{7c}$$

$$W_{i+2l}^{j+8l} = \sum_{\lambda=0}^{1}\sum_{\mu=0}^{1} W_{2i-\lambda}^{2j-\mu}\alpha_{2i-\lambda}\beta_{2j-\mu}. \tag{7d}$$

The expressions (7) and (6a) form a system which enables us to calculate $W_i^j\binom{j=1,\ldots,16l}{i=1,\ldots,4l}$.

2. Calculation of P_m

1. If we remember that a 'deformation or transformation stacking fault' changes the arrangements (h or k) of the layer in which it occurs and of the next layer (Gevers, 1954*a*), we may remark that the last layer of each of the arrangements

$$a_r^s(\ldots{}^{CC}_{hh}),\ a_r^{s+12l}(\ldots{}^{FF}_{hh}),\ a_{r+l}^{s}(\ldots{}^{CC}_{kh}),\ a_{r+l}^{s+12l}(\ldots{}^{FF}_{kh}),$$
$$a_{r+2l}^{s+4l}(\ldots{}^{FC}_{hk}),\ a_{r+2l}^{s+8l}(\ldots{}^{CF}_{hk}),\ a_{r+3l}^{s+4l}(\ldots{}^{FC}_{kk}),$$
$$a_{r+3l}^{s+8l}(\ldots{}^{CF}_{kk})\binom{s=1,\ldots,4l}{r=1,\ldots,l},$$

is h-arranged with its two predecessors, while in all other arrangements this layer is k-arranged.

2. The layer m can be the last in any one of the following arrangements:

$$(1)\ a_r^s(a_r^{s+12l},\ a_{r+l}^{s},\ a_{r+l}^{s+12l},\ a_{r+2l}^{s+4l},\ a_{r+2l}^{s+8l},\ a_{r+3l}^{s+4l},\ a_{r+3l}^{s+8l})\binom{s=1,\ldots,4l}{r=1,\ldots,l}.$$

Each of these terminates with an h-arranged layer. Layer m will be (like the zero layer) an A layer if layer $(m-2)$ is also an A terminating an arrangement $a_{4r-\varepsilon}^{4s-\nu}(\nu=0,1,2,3)(\varepsilon=0,1,2,3)$, and layer $(m-1)$ terminates an arrangement

$$a_{2r-\varrho}^{2s-\sigma}(a_{2r-\varrho}^{2s+8l-\sigma},\ a_{2r+2l-\varrho}^{2s-\sigma},\ a_{2r+2l-\varrho}^{2s+8l-\sigma},\ a_{2r-\varrho}^{2s+8l-\sigma},\ a_{2r-\varrho}^{2s-\sigma},$$
$$a_{2r+2l-\varrho}^{2s+8l-\sigma},\ a_{2r+2l-\varrho}^{2s-\sigma})\ (\varrho=0 \text{ or } 1 \text{ if } \varepsilon=0,1 \text{ or } 2,3)\ (\sigma=0 \text{ or } 1 \text{ if } \nu=0,1 \text{ or } 2,3).$$

So we have, if we take (5) into account:

$$p_m\binom{s}{r} = \sum_{\varepsilon=0}^{3}\sum_{\nu=0}^{3} p_{m-2}\binom{4s-\nu}{4r-\varepsilon}\cdot(1-\alpha_{4r-\varepsilon})(1-\beta_{4s-\nu})\cdot(1-\alpha_{2r-\varrho})(1-\beta_{2s-\sigma}), \tag{8a}$$

$$p_m\binom{s+12l}{r} = \sum_{\varepsilon=0}^{3}\sum_{\nu=0}^{3} p_{m-2}\binom{4s-\nu}{4r-\varepsilon}\cdot(1-\alpha_{4r-\varepsilon})\beta_{4s-\nu}\cdot(1-\alpha_{2r-\varrho})\beta_{2s+8l-\sigma}, \tag{8b}$$

$$p_m\binom{s}{r+l} = \sum_{\varepsilon=0}^{3}\sum_{\nu=0}^{3} p_{m-2}\binom{4s-\nu}{4r-\varepsilon}\cdot\alpha_{4r-\varepsilon}(1-\beta_{4s-\nu})\cdot(1-\alpha_{2r+2l-\varrho})(1-\beta_{2s-\sigma}), \tag{8c}$$

$$p_m\binom{s+12l}{r+l} = \sum_{\varepsilon=0}^{3}\sum_{\nu=0}^{3} p_{m-2}\binom{4s-\nu}{4r-\varepsilon}\cdot\alpha_{4r-\varepsilon}\beta_{4s-\nu}\cdot(1-\alpha_{2r+2l-\varrho})\beta_{2s+8l-\sigma}, \tag{8d}$$

$$p_m\binom{s+4l}{r+2l} = \sum_{\varepsilon=0}^{3}\sum_{\nu=0}^{3} p_{m-2}\binom{4s-\nu}{4r-\varepsilon}\cdot(1-\alpha_{4r-\varepsilon})\beta_{4s-\nu}\cdot\alpha_{2r-\varrho}(1-\beta_{2s+8l-\sigma}), \tag{8e}$$

$$p_m\binom{s+8l}{r+2l} = \sum_{\varepsilon=0}^{3}\sum_{\nu=0}^{3} p_{m-2}\binom{4s-\nu}{4r-\varepsilon}\cdot(1-\alpha_{4r-\varepsilon})(1-\beta_{4s-\nu})\cdot\alpha_{2r-\varrho}\beta_{2s-\sigma}, \tag{8f}$$

$$p_m\binom{s+4l}{r+3l} = \sum_{\varepsilon=0}^{3}\sum_{\nu=0}^{3} p_{m-2}\binom{4s-\nu}{4r-\varepsilon}\cdot\alpha_{4r-\varepsilon}\beta_{4s-\nu}\cdot\alpha_{2r+2l-\varrho}(1-\beta_{2s+8l-\sigma}), \tag{8g}$$

$$p_m\binom{s+8l}{r+3l} = \sum_{\varepsilon=0}^{3}\sum_{\nu=0}^{3} p_{m-2}\binom{4s-\nu}{4r-\varepsilon}\cdot\alpha_{4r-\varepsilon}(1-\beta_{4s-\nu})\cdot\alpha_{2r+2l-\varrho}\beta_{2s-\sigma} \tag{8h}$$

$(r=1,\ldots,l;\ s=1,\ldots,4l;\ \varepsilon=0,1,2,3;\ \nu=0,1,2,3;\ \varrho=0 \text{ or } 1 \text{ if } \varepsilon=0,1 \text{ or } 2,3;$
$\sigma=0 \text{ or } 1 \text{ if } \nu=0,1 \text{ or } 2,3).$

(2) $a_r^{s+4l}(a_r^{s+8l},\ a_{r+l}^{s+4l},\ a_{r+l}^{s+8l},\ a_{r+2l}^{s},\ a_{r+2l}^{s+12l},\ a_{r+3l}^{s},\ a_{r+3l}^{s+12l})\,(^{s=1,\ldots,4l}_{r=1,\ldots,l})$.

Each of these terminates with a k-arranged layer. Their probabilities

$$W_r^{s+4l}(W_r^{s+8l},\ W_{r+l}^{s+4l},\ W_{r+l}^{s+8l},\ W_{r+2l}^{s},\ W_{r+2l}^{s+12l},\ W_{r+3l}^{s},\ W_{r+3l}^{s+12l})$$

depend on the following possibilities:

(a) the layer m is an A-layer;
(b) layer $(m-1)$ is an A-layer arranged as

$$a_{2r-\lambda}^{2s+8l-\mu}(a_{2r-\lambda}^{2s-\mu},\ a_{2r+2l-\lambda}^{2s+8l-\mu},\ a_{2r+2l-\lambda}^{2s-\mu},\ a_{2r-\lambda}^{2s-\mu},\ a_{2r-\lambda}^{2s+8l-\mu},\ a_{2r+2l-\lambda}^{2s-\mu},\ a_{2r+2l-\lambda}^{2s+8l-\mu})\,(^{\mu=0,1}_{\lambda=0,1})$$

and is followed by a layer m in the desired arrangement $a_r^{s+4l}(\ldots)$;

(c) layer $(m-2)$ is an A-layer arranged as $a_{4r-\varepsilon}^{4s-\nu}$ $(^{\nu=0,1,2,3}_{\varepsilon=0,1,2,3})$
followed by a layer $(m-1)$ arranged as

$$a_{2r-\varrho}^{2s+8l-\sigma}(a_{2r-\varrho}^{2s-\sigma},\ a_{2r+2l-\varrho}^{2s+8l-\sigma},\ a_{2r+2l-\varrho}^{2s-\sigma},\ a_{2r-\varrho}^{2s-\sigma},\ a_{2r-\varrho}^{2s+8l-\sigma},\ a_{2r+2l-\varrho}^{2s-\sigma},\ a_{2r+2l-\varrho}^{2s+8l-\sigma})\,(^{\sigma=0\text{ or }1\text{ if }\nu=0,1\text{ or }2,3}_{\varrho=0\text{ or }1\text{ if }\varepsilon=0,1\text{ or }2,3})$$

and by a layer m arranged in the desired arrangement $a_r^{s+4l}(\ldots)$.

If we take this into account, and also (5), we have:

3. The expressions (8), (9) and (6b) form a linear system which has a solution of the form

$$p_m(^{i}_{i}) = c_0(^{i}_{i}) + \sum_r c_r(^{i}_{i})x_r^m\,, \tag{10a}$$

$$P_m = C_0 + \sum_r C_r x_r^m\,, \tag{10b}$$

where x_r are the roots of a characteristic equation. This equation can be found in the usual way (Gevers, 1952, 1954a) by substitution of the formulae (10) into the system. We obtain then the equation:

$$\det.\ \mathscr{C} = 0\,, \tag{11}$$

where the matrix $\mathscr{C}$ is

$$\mathscr{C} = x^2\mathscr{E} + x\mathscr{D}(\mathscr{G}+\mathscr{H}) + \mathscr{I}(G-H)^2\,, \tag{12}$$

where $\mathscr{D}, \mathscr{E}, \mathscr{I}, \mathscr{G}, \mathscr{H}$ are matrixes of order $16l$, of which the elements are themselves matrixes of order $4l$.

$\mathscr{E}$ is a diagonal matrix with elements equal to E, if E is the unit matrix of order $4l$;

$\mathscr{D}$ is a diagonal matrix with elements $\mathscr{D}_{ii}$ so that:

$$\mathscr{D}_{ii}=G(i=1,\ \ldots,\ 4l),\ \mathscr{D}_{ii}=H(i=4l+1,\ \ldots,\ 8l),$$
$$\mathscr{D}_{ii}=H(i=8l+1,\ \ldots,\ 12l),\ \mathscr{D}_{ii}=G(i=12l+1,\ \ldots,\ 16l)$$

if G and H are the matrices we constructed in our previous article (Gevers, 1954b, §§ 2, 4);

$\mathscr{I}$ is a diagonal matrix with elements equal to $(G-H)(G+H)$;

$$W^{s+4l} = p_m(^{s+4l}_{r}) + \sum_{\lambda=0}^{1}\sum_{\mu=0}^{1} p_{m-1}(^{2s+8l-\mu}_{2r-\lambda})\cdot(1-\alpha_{2r-\lambda})(1-\beta_{2s+8l-\mu}) + \sum_{\varepsilon=0}^{3}\sum_{\nu=0}^{3} p_{m-2}(^{4s-\nu}_{4r-\varepsilon})\cdot(1-\alpha_{4r-\varepsilon})\beta_{4s-\nu}\cdot(1-\alpha_{2r-\varrho})(1-\beta_{2s+8l-\sigma})\,, \tag{9a}$$

$$W_r^{s+8l} = p_m(^{s+8l}_{r}) + \sum_{\lambda=0}^{1}\sum_{\mu=0}^{1} p_{m-1}(^{2s-\mu}_{2r-\lambda})\cdot(1-\alpha_{2r-\lambda})\beta_{2s-\mu} + \sum_{\varepsilon=0}^{3}\sum_{\nu=0}^{3} p_{m-2}(^{4s-\nu}_{4r-\varepsilon})\cdot(1-\alpha_{4r-\varepsilon})(1-\beta_{4s-\nu})\cdot(1-\alpha_{2r-\varrho})\beta_{2s-\sigma}\,, \tag{9b}$$

$$W_{r+l}^{s+4l} = p_m(^{s+4l}_{r+l}) + \sum_{\lambda=0}^{1}\sum_{\mu=0}^{1} p_{m-1}(^{2s+8l-\mu}_{2r+2l-\lambda})\cdot(1-\alpha_{2r+2l-\lambda})(1-\beta_{2s+8l-\mu}) + \sum_{\varepsilon=0}^{3}\sum_{\nu=0}^{3} p_{m-2}(^{4s-\nu}_{4r-\varepsilon})\cdot\alpha_{4r-\varepsilon}\beta_{4s-\nu}\cdot(1-\alpha_{2r+2l-\varrho})(1-\beta_{2s+8l-\sigma})\,, \tag{9c}$$

$$W_{r+l}^{s+8l} = p_m(^{s+8l}_{r+l}) + \sum_{\lambda=0}^{1}\sum_{\mu=0}^{1} p_{m-1}(^{2s-\mu}_{2r+2l-\lambda})\cdot(1-\alpha_{2r+2l-\lambda})\beta_{2s-\mu} + \sum_{\varepsilon=0}^{3}\sum_{\nu=0}^{3} p_{m-2}(^{4s-\nu}_{4r-\varepsilon})\cdot\alpha_{4r-\varepsilon}(1-\beta_{4s-\nu})\cdot(1-\alpha_{2r+2l-\varrho})\beta_{2s-\sigma}\,, \tag{9d}$$

$$W_{r+2l}^{s} = p_m(^{s}_{r+2l}) + \sum_{\lambda=0}^{1}\sum_{\mu=0}^{1} p_{m-1}(^{2s-\mu}_{2r-\lambda})\cdot\alpha_{2r-\lambda}(1-\beta_{2s-\mu}) + \sum_{\varepsilon=0}^{3}\sum_{\nu=0}^{3} p_{m-2}(^{4s-\nu}_{4r-\varepsilon})\cdot(1-\alpha_{4r-\varepsilon})(1-\beta_{4s-\nu})\cdot\alpha_{2r-\varrho}(1-\beta_{2s-\sigma})\,, \tag{9e}$$

$$W_{r+2l}^{s+12l} = p_m(^{s+12l}_{r+2l}) + \sum_{\lambda=0}^{1}\sum_{\mu=0}^{1} p_{m-1}(^{2s+8l-\mu}_{2r-\lambda})\cdot\alpha_{2r-\lambda}\beta_{2s+8l-\mu} + \sum_{\varepsilon=0}^{3}\sum_{\nu=0}^{3} p_{m-2}(^{4s-\nu}_{4r-\varepsilon})\cdot(1-\alpha_{4r-\varepsilon})\beta_{4s-\nu}\cdot\alpha_{2r-\varrho}\beta_{2s+8l-\sigma}\,, \tag{9f}$$

$$W_{r+3l}^{s} = p_m(^{s}_{r+3l}) + \sum_{\lambda=0}^{1}\sum_{\mu=0}^{1} p_{m-1}(^{2s-\mu}_{2r+2l-\lambda})\cdot\alpha_{2r+2l-\lambda}(1-\beta_{2s-\mu}) + \sum_{\varepsilon=0}^{3}\sum_{\nu=0}^{3} p_{m-2}(^{4s-\nu}_{4r-\varepsilon})\cdot\alpha_{4r-\varepsilon}(1-\beta_{4s-\nu})\cdot\alpha_{2r+2l-\varrho}(1-\beta_{2s-\sigma})\,, \tag{9g}$$

$$W_{r+3l}^{s+12l} = p_m(^{s+12l}_{r+3l}) + \sum_{\lambda=0}^{1}\sum_{\mu=0}^{1} p_{m-1}(^{2s+8l-\mu}_{2r+2l-\lambda})\cdot\alpha_{2r+2l-\lambda}\beta_{2s+8l-\mu} + \sum_{\varepsilon=0}^{3}\sum_{\nu=0}^{3} p_{m-2}(^{4s-\nu}_{4r-\varepsilon})\cdot\alpha_{4r-\varepsilon}\beta_{4s-\nu}\cdot\alpha_{2r+2l-\varrho}\beta_{2s+8l-\sigma} \tag{9h}$$

$(r = 1, \ldots, l;\ s = 1, \ldots, 4l;\ \lambda = 0, 1;\ \mu = 0, 1;\ \varepsilon = 0, 1, 2, 3;\ \nu = 0, 1, 2, 3;$
$\varrho = 0$ or 1 if $\varepsilon = 0, 1$ or $2, 3$; $\sigma = 0$ or 1 if $\nu = 0, 1$ or $2, 3$).

$\mathcal{G}$ and $\mathcal{H}$ are obtained if, in the expression for G and H, we change each $(1-\alpha_i)$ into $(1-\beta_i)E$ and each α_i into $\beta_i E$.

4. With the aid of (6*a*) and (7) it can be proved that $C_0 = \frac{1}{3}$ and the C_r's can be calculated by solving the system (2). The values of $P_m (m = 0, 1, \ldots)$ may indeed be calculated directly with the aid of (8), (9) and (6*b*) if we take into account that

$$p_0(i_i^j) = W_i^j \text{ and } p_1(i_i^j) = 0 \; (j: 1, \ldots, 16l; \; i = 1, \ldots, 4l).$$

5. It has been stated and proved (Gevers, 1953*a*, 1954*a*) how the expression

$$\sum_r \frac{C_r(1-x_r^2)}{1-2x_r \cos A_3 + x_r^2}$$

of the formula (1) can be calculated without solving the characteristic equation (11) and the system (2), and how an equivalent equation can be calculated from the measurements of the diffuse X-ray intensity.

6. If there is an 'n-layer influence' for the 'faults of the first type' and an 'm-layer influence' for 'those of the second type', we have supposed that $n = m$. This assumption does not restrict the generality of the calculation, since an 'n-layer influence' can always be reduced to an '$(n-p)$-layer influence' by taking

$$\alpha_1 = \alpha_2 = \ldots = \alpha_{2p}; \; \ldots; \quad \alpha_{2ip+1} = \alpha_{2ip+2} = \ldots = \alpha_{2(i+1)p}; \; \ldots .$$

3. Special cases

1. Suppose $\beta_1 = \beta_2 = \ldots = \beta_{16l} = \beta$. This means that the 'deformation or transformation stacking faults' are randomly distributed. With this simple assumption, and making use of the properties of determinants and matrices, we can prove that equation (11) can then be brought into the form

$$\text{det. } C_1 = 0 \text{ if } C_1 = x^2E + xG + [1-3\beta(1-\beta)](G-H)(G+H) . \quad (13)$$

It is easily verified that the formulae given by Wilson (1942), Hendricks & Teller (1942) ($\beta = 0$, $n = 2$), Jagodzinski (1949) ($\beta = 0$, $n = 3$), (Gevers (1952) ($\beta = 0$, special cases $n = 4$ and $n = 6$), Gevers (1954*a*) ($\beta = 0$, $n = 4$), Kakinoki & Komura (1952) ($\beta = 0$, $n =$ any number), Gevers (1954*b*) ($\beta = 0$, $n =$ any number), Paterson (1952) ($\beta \neq 0$, $n = 2$, $\alpha = 1$), Gevers (1953*b*, 1954*a*) ($\beta \neq 0$, $n = 2$), Gevers (1954*a*) ($\beta \neq 0$, $n = 3$, $\alpha_1 = 1$, $\alpha_2 = 0$), Gevers (1954*a*) ($\beta \neq 0$, $n = 4$, $\alpha_2 = 1$, $\alpha_3 = 1$, $\alpha_4 = 0$) and Gevers (1953*c*) ($\beta \neq 0$, $n = 6$, $\alpha_6 = \alpha_7 = \alpha_{11} = 1$, $\alpha_2 = \alpha_{14} = 0$) can be calculated with the aid of (13).

2. If the original pattern (and by this we mean the pattern as it was before the introduction of the 'deformation stacking faults') is a cubic or hexagonal close-packed one with randomly distributed 'growth stacking faults', it can be proved that equation (11) can be brought into the form:

$$\text{det. } C_2 = 0 \text{ if } C_2 = x^2E' + xD'(G'+H') + (2\alpha-1)(G'-H')^2 \quad (14)$$

or

$$\text{det. } C_3 = 0 \text{ if } C_3 = x^2E' + x\alpha(G'+H') + (2\alpha-1)(\varepsilon G' + \varepsilon^* H')(\varepsilon^* G + \varepsilon H') \; (\varepsilon = \exp[-i\tfrac{2}{3}\pi]) , \quad (15)$$

where E', D', G', H' are matrices of order $16l$;

E' is the unit matrix;

D' is the diagonal matrix with $D'_{ii} = \alpha; 1-\alpha; 1-\alpha; \alpha$ for $i = 1, \ldots, 4l; 4l+1, \ldots, 8l; 8l+1, \ldots, 12l; 12l+1, \ldots, 16l$);

G' and H' are constructed as $\mathcal{G}$ and $\mathcal{H}$, but the elements $(1-\beta_i)E$ and $\beta_i E$ have to be changed into $1-\beta_i$ and β_i.

3. We consider now the important case of a cubic close-packed crystal containing 'deformation or transformation stacking faults' (with a general 'n-layer influence'). The characteristic equation is given by (15), making $\alpha = 1$. We can prove that this equation can be split into the two equations det. $C_3' = 0$ and det. $C_3'' = 0$ if

$$C_3' = xE' - \varepsilon G' - \varepsilon^* H' \quad (16a)$$

and

$$C_3'' = xE' - \varepsilon^* G' - \varepsilon H' . \quad (16b)$$

The roots of (16*a*) and (16*b*) will be:

$$x_r = \varrho_r \exp(\pm i\theta_r) , \quad (17a)$$

and we can put

$$C_r = A_r \pm iB_r . \quad (17b)$$

In this case the X-ray intensity I is not given by formula (1). Jagodzinski (1949) considered only the case in which the probabilities (P_m^B and P_m^C) of two layers, m layers apart, being in the relationship $A(B, C) \ldots B(C, A)$ or $A(B, C) \ldots C(A, B)$, are equal, while this is obviously not so in the case we are considering.

We can, however, prove that P_m^B (and P_m^C) are given by (10*b*) and (17*a*) if $m\theta$ is changed into $(m\theta - \frac{2}{3}\pi)$ and $(m\theta + \frac{2}{3}\pi)$. It is easily verified that this is so in the simple case which Paterson (1952) considered.

By generalizing Paterson's (1952) method of calculating I, we obtain

$$I = |F|^2 \frac{\sin^2 \frac{1}{2}N_1A_1}{\sin^2 \frac{1}{2}A_1} \cdot \frac{\sin^2 \frac{1}{2}N_2A_2}{\sin^2 \frac{1}{2}A_2} \left\{ \frac{1+2Q}{3} \cdot \frac{\sin^2 \frac{1}{2}N_3A_3}{\sin^2 \frac{1}{2}A_3} + (1-Q) \sum_r \frac{N_3[A_r(1-\varrho_r^2) \pm 2B_r \sin(A_3 \pm \theta_r)]}{1-2\varrho_r \cos(A_3 \pm \theta_r) + \varrho_r^2} \right\} \quad (18)$$

$$\pm \text{for } H-K = \pm 1 \text{ (mod. 3)} .$$

The relations between the hexagonal indices H, K, L ($A_1 = 2\pi H$, $A_2 = 2\pi K$, $A_3 = \frac{2}{3}\pi L$) and the usual cubic indices h, k, l are given by Paterson (1952).

4. I is given by formula (1) except when 'faults of the second type' are introduced into a regular pattern for which $P_m^B \neq P_m^C$.

This was so in the case considered in 3, but also occurs when the regular stacking is of the SiC 15R-type (*hkkhk*-type). The calculations for the latter case

have also been done on the simple assumption $\beta_1 = \beta_2 = \ldots = \beta$ (Gevers, 1953*c*).

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Some Calculations of Atomic Form Factors*

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X-ray atomic form factors for carbon, nitrogen and oxygen have been computed from Hartree–Fock radial wave functions, and compared with the values previously obtained by James & Brindley, and McWeeny.

The X-ray form factor for coherent radiation is given by

$$f(\mathbf{s}) = \int \varrho(\mathbf{r}) \exp\left[i\mathbf{s}\cdot\mathbf{r}\right] dv_{\mathbf{r}}\,, \tag{1}$$

where $\varrho(\mathbf{r})$ is the electronic density of the isolated atom and $s = 4\pi\lambda^{-1}\sin\theta$ is the magnitude of the vector $\mathbf{s}$ in reciprocal space. If the electronic density is spherically symmetric (1) reduces to

$$f(s) = \int_0^\infty U(r)\frac{\sin sr}{sr}\,dr\,, \tag{2}$$

where $U(r)$ is the total radial charge density. James & Brindley (1931) (J & B) evaluated (2) for a number of atoms, using the Hartree values of $U(r)$ (self-consistent field, without exchange). For other atoms, for which the Hartree field was not available, they resorted to an interpolation. These calculations have been extended to higher values of s by Viervoll & Ögrim (1949).

If the electronic density is aspherical, it is convenient to decompose (1) into the separate electronic contributions. Filled or half-filled sub-shells are spherically symmetric and can be treated as in (2), but odd p electrons, d electrons, etc. require special handling: For a p electron defined by

$$\varrho_p = \left|\sqrt{\left(\frac{3}{4\pi}\right)}\frac{P(r)}{r}\cos\theta\right|^2 \tag{3}$$

(where θ is the polar angle relative to the axis of the orbital and $\int_0^\infty P^2(r)\,dr = 1$), McWeeny (1951) (McW) has shown that the transform of (3) by (1) gives

$$f_p = f_p^{\parallel}\cos^2\Theta + f_p^{\perp}\sin^2\Theta\,, \tag{4}$$

where Θ is the angle between $\mathbf{s}$ and the axis of the orbital and

$$f_p^{\parallel} = \frac{3}{4\pi}\iiint P^2(r)\cos^2\theta\sin\theta\exp\left[isr\cos\theta\right]dr\,d\theta\,d\varphi\,, \tag{5}$$

$$f_p^{\perp} = \frac{3}{4\pi}\iiint P^2(r)\sin^3\theta\exp\left[isr\cos\theta\right]\sin^2\varphi\,dr\,d\theta\,d\varphi\,. \tag{6}$$

McWeeny also obtains a 'mean contribution' by averaging (4) over all directions:

$$\bar{f_p} = \tfrac{1}{3}f_p^{\parallel} + \tfrac{2}{3}f_p^{\perp}\,. \tag{7}$$

Similar quantities $f^{\parallel}, f^{\perp}$ and $\bar{f}$ are defined for the whole atom by addition of the respective contributions of the individual electrons. McWeeny has applied these results to atoms from hydrogen to neon, using the approximate variational wave functions obtained in analytic form for the ground states by Duncanson & Coulson (1944).

Self-consistent fields, many of which even include exchange (the Hartree–Fock calculation), are now

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