other two chelate rings are arranged in the crystal in such a manner as to prevent the existence of a similar lattice wave or mode. The reproducibility of the diffuse patterns with temperature cycling together with the packing arrangement suggest the interpretation that the large anisotropic temperature parameters arise from the thermal motion rather than a slight disorder in the molecular packing is correct.

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Diffraction by a One-Dimensionally Disordered Crystal. I. The Intensity Equation

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The intensity equation $I(\varphi)=N\,\text{spur}\,\mathbf{VF}+\sum_{m=1}^{N-1}(N-m)\,\text{spur}\,\mathbf{VFQ}^m+\text{conj.}$ for X-rays diffracted by a one-dimensionally disordered crystal has been solved by three methods, *viz.* (i) by using the inverse matrix $(\mathbf{1}-\mathbf{Q})^{-1}$, (ii) by diagonalizing $\mathbf{Q}$ by the similarity transformation $\mathbf{OQO}^{-1}$ and by using the solutions of a characteristic equation $\det(y\mathbf{1}-\mathbf{Q})=0$ and a set of simultaneous equations with respect to b_ν's, $\sum_{\nu=1}^{R} b_\nu^\nu y_\nu^m = B_m = \text{spur}\ \mathbf{VFQ}^m$ $(m=0, 1, \cdots, R-1)$, and (iii) by using B_m and the relation between roots and coefficients of the characteristic equation without solving these equations explicitly. These methods should be applied to the problem only after the order of matrices has been reduced to lower order by considering the symmetry character involved in the matrices.

Explicit expressions are given for three cases, namely the case of different thickness, that of equal thickness, and that of displacement stacking faults. In the case of displacement stacking faults, the three-dimensional Patterson function is given with respect to the distribution of origins of layers. The result is compared with that obtained by Allegra.

Introduction

The intensity of X-rays diffracted by a one-dimensionally disordered crystal such as SiC, $CdBr_2$, CdI_2, some alloys of the Laves phase, many other alloys and metals showing the stacking faults between cubic and hexagonal close-packed structures, and some kinds of antiphase domain structures and minerals, has been studied by many researchers, for example, Wilson (1942, 1943), Hendricks & Teller (1942), Zachariasen (1947), Jagodzinski (1949 *a*, *b*, *c*, 1954), Méring (1949), Paterson (1952), Kakinoki & Komura (1952; 1954 *a*, *b*), Gevers

(1952; 1954 *a*, *b*), Warren & Warekois (1955), and Warren (1959).

Of the intensity equations given by them, the most general one, in a matrix form, was given first by Hendricks & Teller (1942) and also by Kakinoki & Komura (1952). It is

$$I(\varphi)=NB_0+\sum_{m=1}^{N-1}(N-m)B_m+\text{conj.},\quad B_m=\text{spur }\mathbf{VFQ}^m\,. \tag{1}$$

This can be rewritten, in its special cases mentioned below,

$$I(\varphi)=NJ_0+\sum_{m=1}^{N-1}(N-m)e^{-im\varphi}J_m+\text{conj.},\quad J_m=\text{spur }\mathbf{VFP}^m \tag{2}$$

or

$$I(\varphi)=V_0V_0^*\{N+\sum_{m=1}^{N-1}(N-m)e^{-im\varphi}T_m+\text{conj.}\},\quad T_m=\text{spur }\boldsymbol{\varepsilon}\mathbf{FP}^m \text{ and } T_0=1 \tag{3}$$

when the intensity is expressed in electron units. The notation in equations (1), (2) and (3) is as follows:

N is the number of layers;
$\varphi=2\pi\zeta$;
$(\mathbf{s}-\mathbf{s}_0)/\lambda=\xi\mathbf{a}^*+\eta\mathbf{b}^*+\zeta\mathbf{c}^*$ (scattering vector);
$\mathbf{s}_0$ and $\mathbf{s}$ are unit vectors along the incident and the scattered directions, respectively;
$\mathbf{a}$ and $\mathbf{b}$ lie in the layer and $\mathbf{c}$ is normal to it;
conj. means the complex conjugate of the foregoing term;

and $\mathbf{V}$, $\mathbf{F}$, $\mathbf{P}$, $\boldsymbol{\varepsilon}$ and $\mathbf{Q}$ are such matrices as

$$\left.\begin{array}{l}(\mathbf{V})_{ji}=V_iV_j^* \quad\text{and}\quad (\mathbf{F})_{ij}=f_i\delta_{ij}\\ \quad\therefore\ (\mathbf{VF})_{ji}=f_iV_iV_j^*\\ (\mathbf{P})_{ij}=P_{ij}\quad\text{and}\quad(\boldsymbol{\Phi})_{ij}=e^{-i\varphi_i}\delta_{ij}\\ \quad\therefore\ (\mathbf{Q})_{ij}=(\boldsymbol{\Phi}\mathbf{P})_{ij}=P_{ij}e^{-i\varphi_i}\end{array}\right\} \tag{4}$$

$$\left.\begin{array}{l}(\boldsymbol{\varepsilon})_{ji}=\varepsilon_i\varepsilon_j^*\\ \quad\left\{\begin{array}{l}\varepsilon_i=\exp\{2\pi i(u_i\xi+v_i\eta)\}\\ \mathbf{u}_i=u_i\mathbf{a}+v_i\mathbf{b}\end{array}\right.\end{array}\right\} \tag{5}$$

where

δ_{ij} is Kronecker's delta;
V_i is the layer form factor of the layer i;
f_i is the probability of finding the layer i at any position and hereafter simply called the existence probability of V_i;
P_{ij} is the probability of finding the layer j after the layer i and hereafter simply called the continuing probability of V_j after V_i;
φ_i is the phase shift due to the thickness of the layer i.

Equation (1) differs from equation (2) with respect to the point that the thicknesses of layers are different from each other for the former while they are all the same for the latter. In the former case, denoting the thicknesses of a standard layer and the layer i by $\mathbf{c}$ and $\mathbf{c}_i$, respectively, $\mathbf{c}_i$ can be expressed

$$\mathbf{c}_i=\mu_i\mathbf{c} \tag{6}$$

and hence the parameters ζ and ζ_i along $\mathbf{c}^*$ and $\mathbf{c}_i^*$, respectively, are connected with each other by

$$\zeta_i=\mu_i\zeta \tag{7}$$

from which

$$\varphi_i=2\pi\zeta_i=2\pi\mu_i\zeta=\mu_i\varphi\,. \tag{8}$$

In the latter case μ_i is always unity and hence

$$\boldsymbol{\Phi}=e^{-i\varphi}\mathbf{I},\quad \mathbf{Q}=e^{-i\varphi}\mathbf{P} \tag{9}$$

where $\mathbf{I}$ is a unit matrix. Therefore equation (1) can be rewritten as equation (2).

As in the case of the stacking faults between cubic and hexagonal close-packed structures, when the atomic arrangements within the layers are all the same but their origins are shifted by vectors $\mathbf{u}_i$ parallel to the layer, V_i can be expressed

$$V_i=V_0\exp\{2\pi i(u_i\xi+v_i\eta)\}=V_0\varepsilon_i \tag{10}$$

where V_0 is the layer form factor for the atomic arrangement common to them. In such a case equation (2) can be rewritten as equation (3).

For convenience, the three cases corresponding to equations (1), (2) and (3) will be hereafter called the cases of different thickness, equal thickness, and displacement stacking faults, respectively.

For the existence probabilities f_i and the continuing probabilities P_{ij} there should be such relations as

$$\sum_{i=1}^{r}f_i=1,\quad \sum_{j=1}^{r}P_{ij}=1\,,\quad \sum_{i=1}^{r}f_iP_{ij}=f_j \tag{11}$$

where r is the number of kinds of layer. If we introduce

$$(\mathbf{M})_{ij}=1\,,\quad (\mathbf{H})_{ij}=(\mathbf{MF})_{ij}=f_j$$

the relations in equation (11) are included in the following matrix relations:

$$\text{spur }\mathbf{H}=\text{spur }\mathbf{F}=1\,,\quad \mathbf{PM}=\mathbf{M}\,,\quad \mathbf{HP}=\mathbf{H}\,. \tag{12}$$

Of these relations the last is important as it shows the consistent relations between f_i's and P_{ij}'s and hence f_i's can be expressed in terms of P_{ij}'s.

The intensity equations (1), (2) and (3) are valid not only for the case where there are faults in the stacking of layers, but also for the case where there is no faulting and hence the crystal has a regular periodicity, each P_{ij}, in such a case, being either 1 or 0. It is important to examine all possible kinds of regular structure which can be derived from any set of P_{ij}'s.

As was done by Jagodzinski (1949), the 'Reichweite' is defined to be s when the continuing probability P_{ij} depends not only on the layer i but also on the combinations of the preceding s layers including the layer i. Equations (1), (2) and (3) were derived first for the case of $s=1$, but, as we have shown, they are also valid for the case of any values of s. When $s=0$ we have only to put $\mathbf{P}=\mathbf{H}$ (Kakinoki & Komura, 1952), and when $s\geq 2$ we have only to divide layers belonging to V_i into $l=r^{s-1}$ subgroups according to the combinations of $(s-1)$ antecedent layers before V_i. Corresponding to such an extension, the order of matrices increases from r to $R=rl=r^s$ and they are expressed

$$\mathbf{V}=\begin{pmatrix} V_1^*V_1\mathbf{M}_l & V_1^*V_2\mathbf{M}_l \ldots\ldots & V_1^*V_r\mathbf{M}_l \\ V_2^*V_1\mathbf{M}_l & V_2^*V_2\mathbf{M}_l \ldots\ldots & V_2^*V_r\mathbf{M}_l \\ \vdots & \vdots & \vdots \\ V_r^*V_1\mathbf{M}_l & V_r^*V_2\mathbf{M}_l \ldots\ldots & V_r^*V_r\mathbf{M}_l \end{pmatrix}_R \quad (\mathbf{M}_l)_{ij}=1$$

$$\mathbf{F}=\begin{pmatrix} f_1 & & & \\ & f_2 & & \\ & & \ddots & \\ & & & f_R \end{pmatrix}_R = \begin{pmatrix} \mathbf{F}_1 & & & \\ & \mathbf{F}_2 & & \\ & & \ddots & \\ & & & \mathbf{F}_r \end{pmatrix}_R,$$

$$\mathbf{\Phi}=\begin{pmatrix} e^{-i\varphi_1}\mathbf{l}_l & & & \\ & e^{-i\varphi_2}\mathbf{l}_l & & \\ & & \ddots & \\ & & & e^{-i\varphi_r}\mathbf{l}_l \end{pmatrix}_R$$

$$\mathbf{P}=\begin{pmatrix} P_{11}\,P_{12} \ldots\ldots & P_{1R} \\ P_{21}\,P_{22} \ldots\ldots & P_{2R} \\ \vdots \quad \vdots & \vdots \\ P_{R1}P_{R2} \ldots\ldots & P_{RR} \end{pmatrix}_R = \begin{pmatrix} \mathbf{P}_{11}\mathbf{P}_{12} \ldots\ldots & \mathbf{P}_{1r} \\ \mathbf{P}_{21}\mathbf{P}_{22} \ldots\ldots & \mathbf{P}_{2r} \\ \vdots \quad \vdots & \vdots \\ \mathbf{P}_{r1}\mathbf{P}_{r2} \ldots\ldots & \mathbf{P}_{rr} \end{pmatrix}_R . \quad (13)$$

For details, the original paper (Kakinoki & Komura (1954*a*) should be referred to.

The present paper will show, in a general form, three methods of solution for the intensity equations (1), (2) and (3). They can be applied to many kinds of stacking fault problems found in, for example, stacking faults between cubic and hexagonal close-packed sructures, Laves phases, anti-phase domain structures, some kinds of martensitic transformation, minerals, *etc.* But individual applications will be successively reported later and hence the present paper is a general introduction to them.

The first method of solution

As was shown by Kakinoki & Komura (1952) and later noted by Allegra (1961), if $\det(\mathbf{l}-\mathbf{Q})\neq 0$ there should be an inverse matrix $(\mathbf{l}-\mathbf{Q})^{-1}$, the ij element of which is $N_{ji}/\det\,(\mathbf{l}-\mathbf{Q})$ where N_{ji} is the cofactor of the ji element of $\det\,(\mathbf{l}-\mathbf{Q})$. In such a case equation (1) becomes

$$I(\varphi)=ND(\varphi)+H(\varphi) \qquad (14a)$$

$$\begin{cases} D(\varphi)=D'(\varphi)+\text{conj.}-B_0 & (14b) \\ \quad D'(\varphi)=\text{spur }\mathbf{VF}(\mathbf{l}-\mathbf{Q})^{-1} & (14c) \\ H(\varphi)=\text{spur }\mathbf{VF}(\mathbf{Q}^{N+1}-\mathbf{Q})\,(\mathbf{l}-\mathbf{Q})^{-2}+\text{conj.} & (14d) \end{cases}$$

where $D(\varphi)$ is the diffuse term and $H(\varphi)$ the higher term which can be usually neglected except for the case when N is very small and φ is near the maximum of $D(\varphi)$ (Méring 1949; Kakinoki & Komura, 1952). If each P_{ij} is 0 or 1 and hence the crystal has a regular periodicity, $D(\varphi)=0$ and $H(\varphi)$ becomes the Laue function.

$D'(\varphi)$ in equation (14*c*) can be further calculated as

$$D'(\varphi)=\frac{\text{spur }\mathbf{VFN}}{\det(\mathbf{l}-\mathbf{Q})}=\sum_{i=1}^{R}\sum_{j=1}^{R} f_iV_iV_j^*N_{ji}/\det(\mathbf{l}-\mathbf{Q}) \qquad (15a)$$

$$=\frac{1}{\det(\mathbf{l}-\mathbf{Q})}\left\{V_1^*\begin{pmatrix} f_1V_1 & f_2V_2 \ldots\ldots & f_RV_R \\ -Q_{21} & 1-Q_{22} \ldots\ldots & -Q_{2R} \\ \vdots & \vdots & \vdots \\ -Q_{R1} & -Q_{R2} \ldots\ldots & 1-Q_{RR} \end{pmatrix} + V_2^*\begin{pmatrix} 1-Q_{11} & -Q_{12} \ldots\ldots & -Q_{1R} \\ f_1V_1 & f_2V_2 \ldots\ldots & f_RV_R \\ \vdots & \vdots & \vdots \\ -Q_{R1} & -Q_{R2} \ldots\ldots & 1-Q_{RR} \end{pmatrix} + \ldots\ldots\right\} \qquad (15b)$$

where $\qquad (\mathbf{N})_{ij}=N_{ji}\,. \qquad (16)$

For the cases of equal thickness and displacement stacking faults $(\mathbf{l}-\mathbf{Q})^{-1}$ becomes

$$(\mathbf{l}-\mathbf{Q})^{-1}=e^{i\varphi}(e^{i\varphi}\mathbf{l}-\mathbf{P})^{-1} \qquad (17)$$

and hence $D(\varphi)$ and $H(\varphi)$ become

$$\begin{cases} D(\varphi)=e^{i\varphi}\text{ spur }\mathbf{VF}(e^{i\varphi}\mathbf{l}-\mathbf{P})^{-1}+\text{conj.}-J_0 \\ H(\varphi)=\text{spur }\mathbf{VF}(e^{-iN\varphi}\mathbf{P}^{N+1}-\mathbf{P})e^{i\varphi}(e^{i\varphi}\mathbf{l}-\mathbf{P})^{-2}+\text{conj.} \end{cases} \qquad (18)$$

for the case of equal thickness and

$$\begin{cases} D(\varphi)=V_0V_0^*\{e^{i\varphi}\text{ spur }\boldsymbol{\varepsilon}\mathbf{F}(e^{i\varphi}\mathbf{l}-\mathbf{P})^{-1}+\text{conj.}-1\} \\ H(\varphi)=V_0V_0^*\{\text{spur }\boldsymbol{\varepsilon}\mathbf{F}(e^{-iN\varphi}\mathbf{P}^{N+1}-\mathbf{P})e^{i\varphi}(e^{i\varphi}\mathbf{l}-\mathbf{P})^{-2} \\ \quad +\text{conj.}\} \end{cases} \qquad (19)$$

for the case of displacement stacking faults.

The second method of solution

As was done by Hendricks & Teller (1942), if we find such matrices $\mathbf{O}$ and $\mathbf{O}^{-1}$ as diagonalizing $\mathbf{Q}$ by the similarity transformation

$$\mathbf{OQO}^{-1}=\mathbf{Q}_0 \quad \text{where} \quad (\mathbf{Q}_0)_{\mu\nu}=y_\nu\delta_{\mu\nu}$$

then $B_m=\text{spur }\mathbf{VFQ}^m$ in equation (1) becomes

$$B_m=\text{spur }\mathbf{VFQ}^m=\sum_{\nu=1}^{R}(\mathbf{OVFO}^{-1})_{\nu\nu}y_\nu^m$$

where y_ν is the νth root of a characteristic equation

$$\det\,(y\mathbf{l}-\mathbf{Q})=0\,. \qquad (20)$$

Hendricks & Teller calculated all elements in **O** and $\mathbf{O}^{-1}$ in their example of graphite but this procedure is laborious. In practice, however, it is unnecessary to find them because if we put $(\mathbf{OVFO}^{-1})_{\nu\nu}=b_\nu$,

$$B_m=\sum_{\nu=1}^{R} b_\nu y_\nu^m \tag{21}$$

and b_ν can be obtained by solving a set of simultaneous equations

$$\begin{aligned} b_1+ \quad b_2+\ldots+ \quad b_R&=B_0 &&=\text{spur}\,\mathbf{VF}\\ y_1b_1+ \quad y_2b_2+\ldots+ \quad y_Rb_R&=B_1 &&=\text{spur}\,\mathbf{VFQ}\\ &\vdots\\ y_1^{R-1}b_1+y_2^{R-1}b_2+\ldots+y_R^{R-1}b_R&=B_{R-1}&&=\text{spur}\,\mathbf{VFQ}^{R-1}. \end{aligned} \tag{22}$$

Finally equation (1) becomes

$$I(\varphi)=NB_0+\sum_{\nu=1}^{R} b_\nu \sum_{m=1}^{N-1}(N-m)y_\nu^m+\text{conj.}=ND(\varphi)+H(\varphi) \tag{23a}$$

$$\left\{\begin{aligned} D(\varphi)&=D'(\varphi)+\text{conj.}-B_0 && (23b)\\ D'(\varphi)&=\sum_{\nu=1}^{R}\frac{b_\nu}{1-y_\nu} && (23c)\\ H(\varphi)&=\sum_{\nu=1}^{R}\frac{b_\nu y_\nu(y_\nu^N-1)}{(1-y_\nu)^2}+\text{conj.} && (23d) \end{aligned}\right.$$

Since y_ν and b_ν are generally complex numbers, they are conveniently put in the forms

$$y_\nu=y_{\nu0}e^{i\delta_\nu} \quad\text{and}\quad b_\nu=b_{\nu0}e^{i\varrho_\nu} \tag{24}$$

where $y_{\nu0}$ and $b_{\nu0}$ are absolute values of y_ν and b_ν, respectively. By noting that $B_0=\sum_{\nu=1}^{R} b_{\nu0}\cos\varrho_\nu$, we can express equations (23b) and (23d) as

$$\left\{\begin{aligned} D(\varphi)&=\sum_{\nu=1}^{R} b_{\nu0}D_\nu(\varphi)\\ H(\varphi)&=\sum_{\nu=1}^{R} b_{\nu0}(H_\nu^{(1)}\cos\varrho_\nu+H_\nu^{(2)}\sin\varrho_\nu) \end{aligned}\right. \tag{25a}$$

where

$$D_\nu(\varphi)=\frac{(1-y_{\nu0}^2)\cos\varrho_\nu-2y_{\nu0}\sin\delta_\nu\sin\varrho_\nu}{1+y_{\nu0}^2-2y_{\nu0}\cos\delta_\nu} \tag{25b}$$

$$\left.\begin{aligned} H_\nu^{(1)}(\varphi)&=2y_{\nu0}[\{2y_{\nu0}-(1+y_{\nu0}^2)\cos\delta_\nu\}(1-y_{\nu0}^N\cos N\delta_\nu)\\ &\quad-(1-y_{\nu0}^2)\sin\delta_\nu\sin N\delta_\nu]\\ &\quad\times(1+y_{\nu0}^2-2y_{\nu0}\cos\delta_\nu)^{-2}.\\ H_\nu^{(2)}(\varphi)&=2y_{\nu0}[y_{\nu0}^N\{2y_{\nu0}-(1+y_{\nu0}^2)\cos\delta_\nu\}\sin N\delta_\nu\\ &\quad+(1-y_{\nu0}^2)\sin\delta_\nu(1-y_{\nu0}^N\cos N\delta_\nu)]\\ &\quad\times(1+y_{\nu0}^2-2y_{\nu0}\cos\delta_\nu)^{-2}, \end{aligned}\right\} \tag{25c}$$

where φ is implicitly included on the right-hand sides through y_ν and b_ν. When equation (20) has equal roots, equation (82) in the Appendix should be used.

Similarly, for the cases of equal thickness and displacement stacking faults, the corresponding equations are as follows.

The case of equal thickness

Characteristic equation:

$$\det(x\mathbf{I}-\mathbf{P})=0 \tag{26}$$

Simultaneous equations for $d_\nu=(\mathbf{OVFO}^{-1})_{\nu\nu}$:

$$\begin{aligned} d_1+ \quad d_2+\ldots+ \quad d_R&=J_0 &&=\text{spur}\,\mathbf{VF}\\ x_1d_1+ \quad x_2d_2+\ldots+ \quad x_Rd_R&=J_1 &&=\text{spur}\,\mathbf{VFP}\\ &\vdots\\ x_1^{R-1}d_1+x_2^{R-1}d_2+\ldots+x_R^{R-1}d_R&=J_{R-1}&&=\text{spur}\,\mathbf{VFP}^{R-1} \end{aligned} \tag{27}$$

$$x_\nu=x_{\nu0}e^{i\delta_\nu}, \quad d_\nu=d_{\nu0}e^{i\varrho_\nu} \tag{28}$$

Intensity equation:

$$I(\varphi)=NJ_0+\sum_{\nu=1}^{R} d_\nu\sum_{m=1}^{N-1}(N-m)x_\nu^m e^{-im\varphi}+\text{conj.}=ND(\varphi)+H(\varphi) \tag{29a}$$

$$\left\{\begin{aligned} D(\varphi)&=D'(\varphi)+\text{conj.}-J_0\\ D'(\varphi)&=\sum_{\nu=1}^{R}\frac{d_\nu e^{i\varphi}}{e^{i\varphi}-x_\nu} && (29b)\\ H(\varphi)&=\sum_{\nu=1}^{R}\frac{d_\nu x_\nu(x_\nu^N-e^{iN\varphi})}{(e^{i\varphi}-x_\nu)^2}e^{-i(N-1)\varphi}+\text{conj.} && (29c) \end{aligned}\right.$$

$$\left\{\begin{aligned} D(\varphi)&=\sum_{\nu=1}^{R} d_{\nu0}D_\nu(\varphi)\\ H(\varphi)&=\sum_{\nu=1}^{R} d_{\nu0}(H_\nu^{(1)}\cos\varrho_\nu+H_\nu^{(2)}\sin\varrho_\nu) \end{aligned}\right. \tag{30a}$$

where

$$D_\nu(\varphi)=\frac{(1-x_{\nu0}^2)\cos\varrho_\nu+2x_{\nu0}\sin(\varphi-\delta_\nu)\sin\varrho_\nu}{1+x_{\nu0}^2-2x_{\nu0}\cos(\varphi-\delta_\nu)} \tag{30b}$$

$$\left.\begin{aligned} H_\nu^{(1)}(\varphi)&=2x_{\nu0}[\{2x_{\nu0}-(1+x_{\nu0}^2)\cos(\varphi-\delta_\nu)\}\\ &\quad\times\{1-x_{\nu0}^N\cos N(\varphi-\delta_\nu)\}\\ &\quad-(1-x_{\nu0}^2)\sin(\varphi-\delta_\nu)\sin N(\varphi-\delta_\nu)]\\ &\quad\times\{1+x_{\nu0}^2-2x_{\nu0}\cos(\varphi-\delta_\nu)\}^{-2}.\\ H_\nu^{(2)}(\varphi)&=-2x_{\nu0}[x_{\nu0}^N\{2x_{\nu0}-(1+x_{\nu0}^2)\cos(\varphi-\delta_\nu)\}\\ &\quad\times\sin N(\varphi-\delta_\nu)+(1-x_{\nu0}^2)\sin(\varphi-\delta_\nu)\\ &\quad\times\{1-x_{\nu0}^N\cos N(\varphi-\delta_\nu)\}]\\ &\quad\times\{1+x_{\nu0}^2-2x_{\nu0}\cos(\varphi-\delta_\nu)\}^{-2}. \end{aligned}\right\} \tag{30c}$$

As can be seen by comparing equations (29a) and (23a), if φ on the right hand sides of equations (30b) and (30c) is put equal to 0, then equations (25b) and (25c) are formally obtained by replacing $x_{\nu0}$ by $y_{\nu0}$. When equation (26) has equal roots, equation (84) in the Appendix should be used.

The case of displacement stacking faults

All equations with c (for d) and T (for J) (31)

which correspond to those from (26) to (30c) except (29a). The corresponding equation to (29a) is

$$I(\varphi)=V_0V_0^*\{N+\sum_{\nu=1}^{R}c_\nu\sum_{m=1}^{N-1}(N-m)x_\nu^m e^{-im\varphi}+\text{conj.}\}$$

$$=V_0V_0^*\{ND(\varphi)+H(\varphi)\} \quad (32)$$

When the characteristic equation has equal roots, equation (85) in the Appendix should be used.

The third method of solution

Using the relations between the roots and the coefficients of the characteristic equation, Gevers (1954a) reduced, in the case of displacement stacking faults, the diffuse term $D(\varphi)$ to a single formula in which unknown x_ν's and c_ν's were eliminated. The same procedure is found to be available even for the general case of different thickness.

The left hand side of the characteristic equation (20) is expanded with respect to y as

$$\det(y\mathbf{l}-\mathbf{Q})=\sum_{n=0}^{R}a_n y^{R-n}=F(y)=\prod_{\nu=1}^{R}(y-y_\nu) \quad (33)$$

where $a_0=1$. If $f_\nu(y)$ is defined as

$$f_\nu(y)=\frac{F(y)}{y-y_\nu}=\sum_{n=0}^{R-1}k_n^{(\nu)}y^{R-n-1}$$

where $k_0^{(\nu)}=1$, then

$$k_n^{(\nu)}=\sum_{m=0}^{n}a_m y_\nu^{n-m}$$

and hence

$$f_\nu(y)=\frac{F(y)}{(y-y_\nu)}=\sum_{n=0}^{R-1}\left(\sum_{m=0}^{n}a_m y_\nu^{n-m}\right)y^{R-n-1}\,. \quad (34)$$

By the use of equations (33), (34) and (21), $D'(\varphi)$ in (23c) and $H(\varphi)$ in (23d) can be transformed as follows:

$$D'(\varphi)=\sum_{\nu=1}^{R}\frac{b_\nu}{1-y_\nu}=\frac{\sum_{\nu=1}^{R}b_\nu f_\nu(1)}{F(1)}=\frac{\sum_{n=0}^{R-1}\sum_{m=0}^{n}a_m\sum_{\nu=1}^{R}b_\nu y_\nu^{n-m}}{\det(\mathbf{l}-\mathbf{Q})}$$

$$\therefore\quad D'(\varphi)=\frac{\sum_{n=0}^{R-1}\sum_{m=0}^{n}a_m B_{n-m}}{\det(\mathbf{l}-\mathbf{Q})}\,. \quad (35)$$

$$H(\varphi)=\sum_{\nu=1}^{R}\frac{b_\nu y_\nu(y_\nu^N-1)}{(1-y_\nu)^2}+\text{conj.}=\sum_{\nu=1}^{R}\frac{-b_\nu y_\nu\sum_{s=0}^{N-1}y_\nu^s}{1-y_\nu}$$

$$+\text{conj.}=\frac{-1}{F(1)}\sum_{\nu=1}^{R}b_\nu y_\nu\left(\sum_{s=0}^{N-1}y_\nu^s\right)f_\nu(1)+\text{conj.}$$

$$\therefore\quad H(\varphi)=\frac{-1}{\det(\mathbf{l}-\mathbf{Q})}\sum_{s=1}^{N}\sum_{n=0}^{R-1}\sum_{m=0}^{n}a_m B_{n-m+s}\,. \quad (36)$$

Equation (35) can be shown to be the same as equation (15a)*.

These equations do not involve unknown quantities such as y_ν and b_ν and hence it is unnecessary to solve both the characteristic equation and the simultaneous equation as was suggested in our preliminary report (Kakinoki & Komura, 1962). Equation (35) is found to hold also when the characteristic equation has equal roots (*e.g.* (88) in the Appendix).

If we put

$$A_n=\sum_{m=0}^{n}a_m B_{n-m}=\sum_{m=0}^{n}a_{n-m}B_m\,, \quad (37)$$

then

$$A_0=B_0 \quad\text{and}\quad A_R=\sum_{m=0}^{R}a_m\sum_{\nu=1}^{R}b_\nu y_\nu^{R-m}$$

$$=\sum_{\nu=1}^{R}b_\nu F(y_\nu)=0\,. \quad (38)$$

Therefore the diffuse term $D(\varphi)=D'(\varphi)+\text{conj.}-B_0$ is rewritten

$$D(\varphi)=\frac{\sum_{n=0}^{R-1}\sum_{m=0}^{R}a_m^*A_n+\text{conj.}-B_0\sum_{n=0}^{R}\sum_{m=0}^{R}a_n a_m^*}{\sum_{n=0}^{R}\sum_{m=0}^{R}a_n a_m^*} \quad (39)$$

or, in another form,

$$D(\varphi)=\frac{D_0+\sum_{p=1}^{R-1}D_p+\text{conj.}}{C_0+\sum_{p=1}^{R}C_p+\text{conj.}} \quad (40)$$

where

$$\begin{cases} C_p=\sum_{n=p}^{R}a_{n-p}a_n^*=\sum_{n=o}^{R-p}a_n a_{n+p}^* & (41a)\\ D_p=\sum_{n=p}^{R}a_n^*A_{n-p}+\sum_{n=p}^{R-1}a_{n-p}A_n^*-C_pB_0\,. & (41b)\end{cases}$$

The following formula is convenient for the calculation of D_p:

$$D_p=\sum_{n=0}^{R-1-p}a_n E_{n+p}, \quad\text{where}\quad E_q=\sum_{m=0}^{R}a_m^*B_{m-q} \quad (41c)$$

with

$$E_R=A_R^*=0,\quad B_{-n}=B_n^*\,,\quad B_R=-\sum_{m=1}^{R}a_m B_{R-m}\,. \quad (41d)$$

E_p's and D_p's for some values of R are listed below:

$$*\sum_{n=0}^{R-1}\sum_{m=0}^{n}a_m B_{n-m}=\sum_{m=0}^{R=1}a_m\sum_{n=0}^{R-1-m}\text{spur}\,\mathbf{VFQ}^n=\sum_{m=0}^{R-1}a_m\,\text{spur}\,\mathbf{VF}(\mathbf{l}$$
$$-\mathbf{Q}^{R-m})(\mathbf{l}-\mathbf{Q})^{-1}=\frac{1}{\det(\mathbf{l}-\mathbf{Q})}\{\text{spur}\,\mathbf{VFN}\sum_{m=0}^{R-1}a_m-\sum_{m=0}^{R-1}a_m\sum_{\nu=1}^{R}$$
$$\times(\mathbf{ONVFO}^{-1})_{\nu\nu}y_\nu{}^{R-m}\}=\frac{1}{\det(\mathbf{l}-\mathbf{Q})}\,[\text{spur}\,\mathbf{VFN}\{\det(\mathbf{l}-\mathbf{Q})-$$
$$a_R\}-\sum_{\nu=1}^{R}(\mathbf{ONVFO}^{-1})_{\nu\nu}(0-a_R)]=\text{spur}\mathbf{VFN}\,.$$

$R=2$

$$E_1=B_1^*+a_1^*B_0+a_2^*B_1$$
$$E_0=B_0+a_1^*B_1+a_2^*B_2=(1-a_2a_2^*)B_0+(a_1^*-a_1a_2^*)B_1. \quad (42a)$$

$$D_1=E_1$$
$$D_0=E_0+a_1E_1=a_1B_1^*+\text{conj.}+(1+a_1a_1^*-a_2a_2^*)B_0\,. \quad (42b)$$

$R=3$

$$E_2=B_2^*+a_1^*B_1^*+a_2^*B_0+a_3^*B_1$$
$$E_1=B_1^*+a_1^*B_0+a_2^*B_1+a_3^*B_2$$
$$E_0=B_0+a_1^*B_1+a_2^*B_2+a_3^*B_3=(1-a_3a_3^*)B_0$$
$$+(a_1^*-a_2a_3^*)B_1+(a_2^*-a_1a_3^*)B_2\,. \quad (43a)$$

$$D_2=E_2$$
$$D_1=E_1+a_1E_2$$
$$D_0=E_0+a_1E_1+a_2E_2$$
$$=a_2B_2^*+\text{conj.}+(a_1+a_2a_1^*)B_1^*+\text{conj.}$$
$$+(1+a_1a_1^*+a_2a_2^*-a_3a_3^*)B_0\,. \quad (43b)$$

$R=4$

$$E_3=B_3^*+a_1^*B_2^*+a_2^*B_1^*+a_3^*B_0+a_4^*B_1$$
$$E_2=B_2^*+a_1^*B_1^*+a_2^*B_0+a_3^*B_1+a_4^*B_2$$
$$E_1=B_1^*+a_1^*B_0+a_2^*B_1+a_3^*B_2+a_4^*B_3$$
$$E_0=B_0+a_1^*B_1+a_2^*B_2+a_3^*B_3+a_4^*B_4$$
$$=(1-a_4a_4^*)B_0+(a_1^*-a_3a_4^*)B_1$$
$$+(a_2^*-a_2a_4^*)B_2+(a_3^*-a_1a_4^*)B_3\,. \quad (44a)$$

$$D_3=E_3$$
$$D_2=E_2+a_1E_3$$
$$D_1=E_1+a_1E_2+a_2E_3$$
$$D_0=E_0+a_1E_1+a_2E_2+a_3E_3$$
$$=a_3B_3^*+\text{conj.}+(a_2+a_3a_1^*)B_2^*+\text{conj.}$$
$$+(a_1+a_2a_1^*+a_3a_2^*)B_1+\text{conj.}$$
$$+(1+a_1a_1^*+a_2a_2^*+a_3a_3^*-a_4a_4^*)B_0\,. \quad (44b)$$

For the case of equal thickness, corresponding equations are similarly calculated to be

$$D'(\varphi)=\frac{\sum_{n=0}^{R-1} e^{-in\varphi}\sum_{m=0}^{n} a_m J_{n-m}}{\sum_{n=0}^{R} a_n e^{-in\varphi}} \quad (45)$$

$$D(\varphi)=\frac{D_0+\sum_{p=1}^{R-1} D_p e^{ip\varphi}+\text{conj.}}{C_0+\sum_{p=1}^{R} C_p e^{ip\varphi}+\text{conj.}} \quad (46)$$

where a_n's are the coefficients in the expansion

$$\det(x\mathbf{I}-\mathbf{P})=\sum_{n=0}^{R} a_n x^{R-n}=\prod_{\nu=1}^{R}(x-x_\nu) \quad (47)$$

and B_n in the corresponding equations should be replaced by J_n.

For the case of displacement stacking faults, all these equations hold if J_n is replaced by T_n.

Fourier transformation

In the present paper the lateral size of the crystal is assumed to be so large that $I(\varphi)$ has not any appreciable value outside $\xi=h$ and $\eta=k$ where h and k are integers. Thus $I(\varphi)$ is a function of h and k through $\mathbf{V}$. In the case of displacement stacking faults a function $I_0(hk\varphi)$ is defined as

$$I_0(hk\varphi)=\frac{I(hk\varphi)}{NV_0V_0^*}$$
$$=1+\sum_{m=1}^{N-1}\left(1-\frac{m}{N}\right)e^{-im\varphi}T_m(hk)+\text{conj.} \quad (48)$$

By Fourier transformation $T_m(hk)$ is given by

$$T_m(hk)=\frac{1}{(1-m/N)}\frac{1}{2\pi}\int_0^{2\pi}I_0(hk\varphi)e^{im\varphi}d\varphi$$
$$=\frac{1}{(1-m/N)}\int_0^1 I_0(hk\zeta)e^{2\pi im\zeta}d\zeta$$
$$T_0(hk)=1=\int_0^1 I_0(hk\zeta)d\zeta \quad (49)$$

in which, when $m \ll N$, m/N can be neglected. On the other hand

$$T_m(hk)=\text{spur }\boldsymbol{\varepsilon}\mathbf{F}\mathbf{P}^m=\sum_{i=1}^{R}\sum_{j=1}^{R}\varepsilon_i\varepsilon_j^*(\mathbf{F}\mathbf{P}^m)_{ij}$$
$$=\sum_{i=1}^{R}\sum_{j=1}^{R}A_{ij}^{(m)}\exp\left[-2\pi i\{(u_j-u_i)h+(v_j-v_i)k\}\right] \quad (50)$$

where

$$A_{ij}^{(m)}=(\mathbf{F}\mathbf{P}^m)_{ij}=\sum_{n_1=1}^{R}\sum_{n_2=1}^{R}\ldots\ldots\sum_{n_{m-1}=1}^{R}f_iP_{in_1}P_{n_1n_2}\ldots.P_{n_{m-1}j}, \quad (51)$$

and this is the probability of finding two layers of i and j at the tth and $(t+m)$th positions respectively.

As was done by Zachariasen (1947), $W_m(uv)$ is defined as the probability of finding two layers separated by m layers such that the relative displacement of the origin of the layer at the $(t+m)$th position to the origin of the layer at the tth position is given by $(u\mathbf{a}+v\mathbf{b}+m\mathbf{c})$. Then $W_m(uv)$ is the three-dimensional Patterson function with respect to the distribution of origins of layers. Since $W_m(uv)$ is periodic with respect to u and v, it can be expanded by a Fourier series such as

$$W_m(uv)=\sum_{h}\sum_{k}{}_{-\infty}^{\infty}\ \omega_{hk}^{(m)}\exp\{2\pi i(hu+kv)\} \quad (52)$$

where $\omega_{00}^{(m)}=1$ because of the normalization condition of $W_m(uv)$. By the use of $W_m(uv)$, $T_m(hk)$ is generally expressed

$$T_m(hk)=\int_0^1\int_0^1 W_m(uv)\exp\{-2\pi i(hu+kv)\}dudv\,. \quad (53)$$

Substituting equation (52) in equation (53), we obtain

$$\omega_{hk}^{(m)}=T_m(hk) \quad\text{and}\quad \omega_{00}^{(m)}=T_m(00)=1\,, \quad (54)$$

because, when $h=0$ and $k=0$, $\varepsilon_i=1$ and $\boldsymbol{\varepsilon}=\mathbf{M}$ and hence

$$T_m(00)=\text{spur }\mathbf{MFP}^m=\text{spur }\mathbf{HP}^m=\text{spur }\mathbf{H}=1$$

from equation (12). Therefore

$$W_m(uv)=\sum_h\sum_k{}_{-\infty}^{\infty}\,T_m(hk)\exp\{2\pi i(hu+kv)\} \quad (55)$$

where $T_m(hk)$ can be obtained from the observed intensity by equation (49), at least when $m\ll N$.

Substituting equation (50) in equation (55), we can calculate

$$W_m(uv)=\sum_{i=1}^{R}\sum_{j=1}^{R}A_{ij}^{(m)}\sum_h\sum_k{}_{-\infty}^{\infty}\exp[2\pi i\{h(u-\overline{u_j-u_i})+k(v-\overline{v_j-v_i})\}]$$

$$=\sum_p\sum_q{}_{-\infty}^{\infty}\{\sum_{i=1}^{R}\sum_{j=1}^{R}A_{ij}^{(m)}\delta(u-\overline{u_j-u_i}-p)\delta(v-\overline{v_j-v_i}-q)\}\,, \quad (56)$$

where p and q are integers and $\delta(x)$ is the delta function which comes from

$$\sum_{h=-\infty}^{\infty}\exp(2\pi ihx)=\sum_{p=-\infty}^{\infty}\delta(x-p)\,.$$

Equation (56) shows the mathematical expression of the definition of $W_m(uv)$ for the case of displacement stacking faults.

Reduction in the order of matrices

In some special problems the matrices used above have a special symmetry with respect to their elements. For example, as was shown by Kakinoki & Komura (1954*b*) and Komura (1962) and will be generally discussed in a later article, in the case of displacement stacking faults between cubic and hexagonal close-packed structures, $\boldsymbol{\varepsilon}$, $\mathbf{F}$ and $\mathbf{P}$ can be expressed as

$$\boldsymbol{\varepsilon}=\begin{pmatrix}\mathbf{M} & \varepsilon^*\mathbf{M} & \varepsilon\mathbf{M}\\ \varepsilon\mathbf{M} & \mathbf{M} & \varepsilon^*\mathbf{M}\\ \varepsilon^*\mathbf{M} & \varepsilon\mathbf{M} & \mathbf{M}\end{pmatrix},\quad \mathbf{F}=\tfrac{1}{3}\begin{pmatrix}\mathbf{W} & & \\ & \mathbf{W} & \\ & & \mathbf{W}\end{pmatrix}.$$

$$\mathbf{P}=\begin{pmatrix}0 & \mathbf{P}_1 & \mathbf{P}_2\\ \mathbf{P}_2 & 0 & \mathbf{P}_1\\ \mathbf{P}_1 & \mathbf{P}_2 & 0\end{pmatrix}. \quad (57)$$

As a result

$$\text{spur }\boldsymbol{\varepsilon}\mathbf{FP}^m=\text{spur }\mathbf{H}(\varepsilon\mathbf{P}_1+\varepsilon^*\mathbf{P}_2)^m\,,\quad \mathbf{H}=\mathbf{MW}\,. \quad (58)$$

In this expression the order of the matrices $\mathbf{M}$, $\mathbf{W}$, $\mathbf{H}$, $\mathbf{P}_1$ and $\mathbf{P}_2$ is a third of that of $\boldsymbol{\varepsilon}$, $\mathbf{F}$ and $\mathbf{P}$. In such a case it is convenient to use

$$\det(x\mathbf{1}-\varepsilon\mathbf{P}_1-\varepsilon^*\mathbf{P}_2)=0 \quad \text{(characteristic equation)} \quad (59)$$

$$\sum_{\nu=1}^{R/3}c_\nu x_\nu^m=T_m=\text{spur }\mathbf{H}(\varepsilon\mathbf{P}_1+\varepsilon^*\mathbf{P}_2)^m \quad \text{(simultaneous equations)} \quad (60)$$

where $c_\nu=(\mathbf{OHO}^{-1})_{\nu\nu}$ instead of equations (26) and (27). Thus, when the matrices have some special symmetry, it is better to apply the method of solution described above to the problem after reducing the matrices to those having lower order.

The fact that such a reduction can be achieved is due to the fact that, as is well known, not the absolute but the relative displacement between any two layers contributes to the diffracted intensity. This was independently pointed out also by Allegra (1961, 1964).

Consider the case in which there are six kinds of layer,

$$V_a=V_1\,,\quad V_b=V_1\varepsilon^*\,,\quad V_c=V_1\varepsilon$$
$$V_A=V_2\,,\quad V_B=V_2\varepsilon^*\,,\quad V_C=V_2\varepsilon \quad (61)$$

where

$$\varepsilon=e^{i\Delta}\quad\text{and}\quad \Delta=2\pi(h-k)/3 \quad (62)$$

as in the example of Komura (1962) and where the continuing probabilities, when $s=2$, are given by:

	c a	B a	b A	C A	a b	C b	c B	A B	b c	A c	a C	B C
ca					α_1						$1-\alpha_1$	
Ba					α_2						$1-\alpha_2$	
bA								α_3		$1-\alpha_3$		
CA								α_4		$1-\alpha_4$		
ab			$1-\alpha_1$						α_1			
Cb			$1-\alpha_2$						α_2			
cB		$1-\alpha_3$										α_3
AB		$1-\alpha_4$										α_4
bc	α_1						$1-\alpha_1$					
Ac	α_2						$1-\alpha_2$					
aC				α_3		$1-\alpha_3$						
BC				α_4		$1-\alpha_4$						

$$=\begin{pmatrix}0 & \mathbf{p}_1 & \mathbf{p}_2\\ \mathbf{p}_2 & 0 & \mathbf{p}_1\\ \mathbf{p}_1 & \mathbf{p}_2 & 0\end{pmatrix}_{12}=\mathbf{P}\,. \quad (63)$$

Then

$$\mathbf{V}=\begin{pmatrix}\mathbf{v} & \varepsilon^*\mathbf{v} & \varepsilon\mathbf{v}\\ \varepsilon\mathbf{v} & \mathbf{v} & \varepsilon^*\mathbf{v}\\ \varepsilon^*\mathbf{v} & \varepsilon\mathbf{v} & \mathbf{v}\end{pmatrix}_{12}$$

$$\mathbf{v}=\begin{pmatrix}V_1^*V_1 & V_1^*V_1 & V_1^*V_2 & V_1^*V_2\\ V_1^*V_1 & V_1^*V_1 & V_1^*V_2 & V_1^*V_2\\ V_2^*V_1 & V_2^*V_1 & V_2^*V_2 & V_2^*V_2\\ V_2^*V_1 & V_2^*V_1 & V_2^*V_2 & V_2^*V_2\end{pmatrix}_4$$

$$\mathbf{F}=\tfrac{1}{3}\begin{pmatrix}\mathbf{f} & & \\ & \mathbf{f} & \\ & & \mathbf{f}\end{pmatrix}_{12}\quad \mathbf{f}=\begin{pmatrix}f_1 & & & \\ & f_2 & & \\ & & f_3 & \\ & & & f_4\end{pmatrix}_4 \quad (64)$$

$$\mathbf{\Phi}=\begin{pmatrix}\boldsymbol{\phi} & & \\ & \boldsymbol{\phi} & \\ & & \boldsymbol{\phi}\end{pmatrix}_{12}$$

$$\boldsymbol{\phi}=\begin{pmatrix}e^{-i\varphi_1} & & & \\ & e^{-i\varphi_1} & & \\ & & e^{-i\varphi_2} & \\ & & & e^{-i\varphi_2}\end{pmatrix}_4$$

$\mathbf{Q}=\mathbf{\Phi P}$.

In such a case, similarly to equation (58),

$$\text{spur }\mathbf{VFQ}^m=\text{spur }\mathbf{vf}(\varepsilon\boldsymbol{\phi}\mathbf{p}_1+\varepsilon^*\boldsymbol{\phi}\mathbf{p}_2)^m=\text{spur }\mathbf{vfQ}'^m \quad (65)$$

where

$$\mathbf{Q}'=\varepsilon\boldsymbol{\phi}\mathbf{p}_1+\varepsilon\boldsymbol{\phi}^*\mathbf{p}_2=$$

$$=\begin{pmatrix}\alpha_1e^{-i\phi_1} & & (1-\alpha_1)e^{-i\phi_3} & \\ \alpha_2e^{-i\phi_1} & & (1-\alpha_2)e^{-i\phi_3} & \\ & (1-\alpha_3)e^{-i\phi_2} & & \alpha_3e^{-i\phi_4} \\ & (1-\alpha_4)e^{-i\phi_2} & & \alpha_4e^{-i\phi_4}\end{pmatrix}_4 \quad (66)$$

and

$$\phi_1=\varphi_1-\Delta\,,\quad \phi_2=\varphi_2+\Delta\,,\quad \phi_3=\varphi_1+\Delta\,,\quad \phi_4=\varphi_2-\Delta\,. \quad (67)$$

Since $\mathbf{v}$ can be factored as

$$\mathbf{v}=$$

$$\begin{pmatrix}V_1^* & & & \\ & V_1^* & & \\ & & V_2^* & \\ & & & V_2^*\end{pmatrix}\begin{pmatrix}1&1&1&1\\1&1&1&1\\1&1&1&1\\1&1&1&1\end{pmatrix}\begin{pmatrix}V_1 & & & \\ & V_1 & & \\ & & V_2 & \\ & & & V_2\end{pmatrix}$$

$$=\mathbf{S}^*\mathbf{MS}\quad\text{(put)} \quad (68)$$

if we define a row vector $\mathbf{V}$ whose elements are V_1, V_1, V_2, V_2 and a column vector $\mathbf{V}^*$ whose elements are V_1^*, V_1^*, V_2^*, V_2^* then

$$\text{spur }\mathbf{vfQ}'^m=\text{spur }\mathbf{MSfQ}'^m\mathbf{S}^*=\mathbf{VfQ}'^m\mathbf{V}^* \quad (69)$$

which is the same as the result obtained by Allegra (1961, 1963). He derived equation (69) with new $\mathbf{Q}'$ without considering the symmetry character of matrices but directly from the fact that

the relative displacement between

$$\underline{c}\underline{a}\ \&\ a\underline{b}\text{ is }\varepsilon^*=e^{-i\Delta}$$
$$a\underline{b}\ \&\ b\underline{c}\text{ is }\varepsilon^*=e^{-i\Delta}$$
$$b\underline{c}\ \&\ c\underline{a}\text{ is }\varepsilon^*=e^{-i\Delta} \quad (70)$$

which are the same and the fact that the intensity contribution from the pair of

$$c\underline{a}\ \&\ a\underline{b}\text{ is }(\underbrace{V_1}_{a})e^{-i\varphi_1}(\underbrace{V_1\varepsilon^*}_{b})^*=V_1V_1^*e^{-i(\varphi_1-\Delta)}$$
$$a\underline{b}\ \&\ b\underline{c}\text{ is }(\underbrace{V_1\varepsilon^*}_{b})e^{-i\varphi_1}(\underbrace{V_1\varepsilon}_{c})^*=V_1V_1^*e^{-i(\varphi-1\Delta)}$$
$$b\underline{c}\ \&\ c\underline{a}\text{ is }(\underbrace{V_1\varepsilon}_{c})e^{-i\varphi_1}(\underbrace{V_1}_{a})^*=V_1V_1^*e^{-i(\varphi_1-\Delta)} \quad (71)$$

which are the same. Such a new definition of $\mathbf{Q}'$ is explicitly presented by Allegra (1961, 1963) but equivalent to equation (58).

Another merit of the new definition of $\mathbf{Q}'$ is as follows: If ϕ_1 and ϕ_2 in equation (66) are defined, differently from equation (67), as

$$\phi_1=\psi_1\,,\quad \phi_2=\psi_2+\Delta'\,,\quad \phi_3=\psi_1+\Delta',\quad \phi_4=\psi_2$$
$$\psi_1=M_1\psi_0\,,\quad \psi_2=M_2\psi_0\,,\quad \Delta'=h\pi,\ k\pi\text{ or }(h+k)\pi \quad (72a)$$

with

$$V_1=\sin\pi M_1\zeta/\sin\pi\zeta\quad\text{and}\quad V_2=\sin\pi M_2\zeta/\sin\pi\zeta\,, \quad (72b)$$

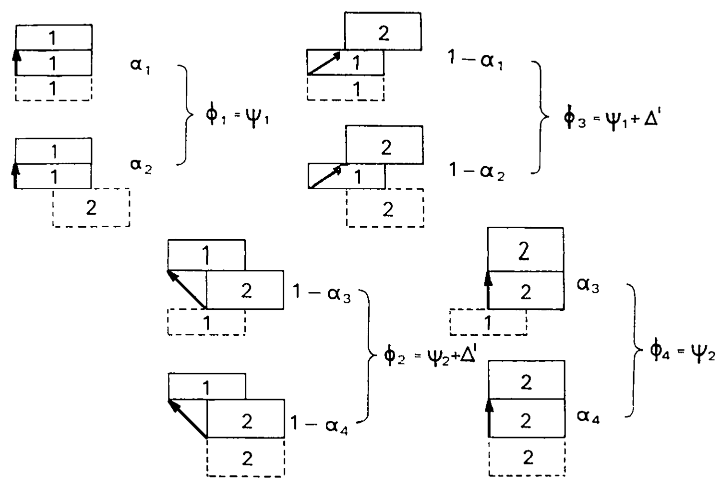

Fig. 1. A kind of anti-phase domain structure. 1 consists of M_1 layers and 2 consists of M_2 layers. The Reichweite $s=2$. The broken lines show the antecedent layers and the thick arrows show the relative displacements between two successive layers. ψ_0, ψ_1 and ψ_2 are perpendicular phase shifts due to the thicknesses of one layer, M_1 layers and M_2 layers respectively. Δ is the parallel phase shift due to anti-phase.

then the intensity equation expressed in terms of V_1, V_2, ϕ_1, ϕ_2 should be the same both for the former and the latter examples. The latter case corresponds to the problem of some kinds of antiphase domain structure as shown in Fig. 1. Thus there are several ways of separating ϕ into the perpendicular part φ and the parallel part Δ, and the same type of intensity equation is applicable to the different problems so long as the types of matrices are the same.

The $\mathbf{Q}_{(H)}$ defined by Hendricks & Teller (1942) is similar in its form to equation (66) but in their case Δ due to the parallel displacement was not considered.

Further remarks

The three types of general method of solution mentioned above should be applied to the intensity equation only after the order of matrices used has been reduced either by the consideration of symmetry character involved or by the new definition of $\mathbf{Q}'$.

In the second method of solution, the diffuse term $D(\varphi)$ is expressed by a sum of ν components of $D_\nu(\varphi)$'s and hence it is convenient for us to know which parameter contributes to which part of the diffuse maxima. But the more the order of matrices increases, the more difficult is it to solve both the characteristic equation and the set of simultaneous equations. Even when it is easy to solve them, if x_ν and c_ν are complicated, it is often difficult to express them in the form of equation (28). In such a case the third method is better because it is unnecessary to solve both equations.

Even when the characteristic equation has equal roots, equations (35), (40), (45) and (46) can be shown to hold (See Appendix).

The term 'Reichweite' may suggest that the interlayer force has an appreciable effect on the s neighbours. This may or may not be true. So far as diffraction analysis is concerned, an appropriate interpretation of the Reichweite is that it is only a parameter to limit the number of configurations by which the observed diffuse intensity can be well explained. What kind of relation exists between the Reichweite and the range of interlayer force is another problem, which may be difficult to solve.

Examples dealt with by the three methods of solution will be reported successively in subsequent papers for problems such as that of the displacement stacking faults between cubic and hexagonal close-packed structures, that between modified close-packed structures (Laves phase, some kinds of martensitic transformation), some kinds of anti-phase domain structure, minerals, *etc.*

APPENDIX

When the characteristic equation has t_ν equal roots, it is given by

$$F(x)=\prod_{\nu=1}^{\sigma}(x-x_\nu)^{t_\nu}=0 \quad \text{where} \quad \sum_{\nu=1}^{\sigma} t_\nu=R\,. \tag{73}$$

In such a case, $\mathbf{OPO}^{-1}=\mathbf{P}_0$ is generally expressed by Jordan's normal form* as

$$\mathbf{P}_0=\begin{pmatrix} \mathbf{p}_1 & & & 0 \\ & \mathbf{p}_2 & & \\ & & \ddots & \\ 0 & & & \mathbf{p}_\sigma \end{pmatrix}_R$$

$$\text{with } \mathbf{p}_\nu=\begin{pmatrix} x_\nu & 1 & & 0 \\ & x_\nu & 1 & \\ & & \ddots & 1 \\ 0 & & & x_\nu \end{pmatrix}_{t_\nu}. \tag{74}$$

If $\mathbf{O\varepsilon FO}^{-1}$ is expressed

$$\mathbf{O\varepsilon FO}^{-1}=\begin{pmatrix} \mathbf{v}_1^{(1)} & \mathbf{v}_1^{(2)} & \cdots & \mathbf{v}_1^{(\sigma)} \\ \mathbf{v}_2^{(1)} & \mathbf{v}_2^{(2)} & \cdots & \mathbf{v}_2^{(\sigma)} \\ \vdots & \vdots & & \vdots \\ \mathbf{v}_\sigma^{(1)} & \mathbf{v}_\sigma^{(2)} & \cdots & \mathbf{v}_\sigma^{(\sigma)} \end{pmatrix}_R$$

where $\mathbf{v}_\nu^{(\mu)}$ is a rectangular matrix with t_ν rows and t_μ columns,

$$T_m=\text{spur }\boldsymbol{\varepsilon}\mathbf{FP}^m=\sum_{\nu=1}^{\sigma}\text{spur }\mathbf{v}_\nu^{(\nu)}\mathbf{p}_\nu^m=\sum_{\nu=1}^{\sigma}T_m^{(\nu)} \tag{75}$$

with $\qquad T_m^{(\nu)}=\text{spur }\mathbf{v}_\nu^{(\nu)}\mathbf{p}_\nu^m\,.$

When $\mathbf{p}_\nu$ is put in the form

$$\mathbf{p}_\nu=x_\nu\mathbf{1}+\mathbf{u}_\nu \quad \text{with} \quad \mathbf{u}_\nu=\begin{pmatrix} 0 & 1 & & 0 \\ & 0 & 1 & \\ & & \ddots & 1 \\ 0 & & & 0 \end{pmatrix}_{t_\nu} \tag{76}$$

where the order of $\mathbf{1}$ and $\mathbf{u}_\nu$ is t_ν, then

$$\mathbf{p}_\nu^m=\sum_{n=0}^{m}{}_mC_n x_\nu^{m-n}\mathbf{u}_\nu^n$$

and hence

$$T_m^{(\nu)}=\begin{cases} \sum_{n=0}^{m} c_\nu^{(n)}\,{}_mC_n x_\nu^{m-n} & \text{for } m\le t_\nu-2 \\ \sum_{n=0}^{t_\nu-1} c_\nu^{(n)}\,{}_mC_n x_\nu^{m-n} & \text{for } m\ge t_\nu-1 \end{cases} \tag{77}$$

where

$$c_\nu^{(n)}=\begin{cases} \text{spur }\mathbf{v}_\nu^{(\nu)}\mathbf{u}_\nu^n & \text{for } n\le t_\nu-1 \\ 0 & \text{for } n\ge t_\nu \end{cases} \tag{78}$$

since $\mathbf{u}_\nu^{t_\nu}=0$. Equation (77) is equivalent to equation (5) in our preliminary report (Kakinoki & Komura, 1962) when $\sigma=1$ and $t_1=3$ and $T_m=\sum_{\nu=1}^{\sigma}T_m^{(\nu)}$ is equivalent to equation (8) in the paper. Thus

* Even when some 1 elements in $\mathbf{p}_\nu$ are 0, the procedure described below is applicable.

$$\sum_{m=0}^{N-1}(N-m)e^{-im\varphi}T_m$$
$$=\sum_{\nu=1}^{\sigma}\sum_{n=0}^{t_\nu-1}c_\nu^{(n)}\sum_{m=n}^{N-1}(N-m)_mC_nx_\nu^{m-n}e^{-im\varphi}$$
$$=\sum_{\nu=1}^{\sigma}\sum_{n=0}^{t_\nu-1}c_\nu^{(n)}\sum_{m=n}^{N-1}(N-m)\frac{m(m-1)\ldots\ldots(m-n+1)}{n!}$$
$$\times x_\nu^{m-n}e^{-im\varphi}=\sum_{\nu=1}^{\sigma}\sum_{n=0}^{t_\nu-1}c_\nu^{(n)}\frac{1}{n!}\frac{\partial^n}{\partial x_\nu^n}\sum_{m=0}^{N-1}(N-m)x_\nu^me^{-im\varphi}$$
$$=\sum_{\nu=1}^{\sigma}\sum_{n=0}^{t_\nu-1}c_\nu^{(n)}\frac{1}{n!}\frac{\partial^n}{\partial x_\nu^n}\left\{\frac{N}{1-x_\nu e^{-i\varphi}}\right.$$
$$\left.+\frac{x_\nu e^{-i\varphi}(x_\nu^Ne^{-iN\varphi}-1)}{(1-x_\nu e^{-i\varphi})^2}\right\}=\sum_{\nu=1}^{\sigma}(ND'_\nu+H'_\nu)$$

where

$$\begin{cases} D'_\nu(\varphi)=\sum_{n=0}^{t_\nu-1}c_\nu^{(n)}\dfrac{e^{i\varphi}}{(e^{i\varphi}-x_\nu)^{1+n}} \\ H'_\nu(\varphi)=\sum_{n=0}^{t_\nu-1}c_\nu^{(n)}\sum_{s=0}^{n} \\ \quad\times\dfrac{(1+n-s)\{_{N+1}C_sx_\nu^{N+1-s}e^{-i(N-1)\varphi}-(x_\nu\delta_{s0}+\delta_{s1})e^{i\varphi}\}}{(e^{i\varphi}-x_\nu)^{n-s+2}}\end{cases}\tag{79}$$

Finally $I(\varphi)$ can be rewritten

$$I(\varphi)=V_0V_0^*\{ND(\varphi)+H(\varphi)\}$$

$$\begin{cases} D(\varphi)=\sum_{\nu=1}^{\sigma}D'_\nu(\varphi)+\text{conj.}-T_0 \\ H(\varphi)=\sum_{\nu=1}^{\sigma}H'_\nu(\varphi)+\text{conj.}\end{cases}\tag{80}$$

For the case of different thickness, as mentioned before, φ has only to be put equal to 0 and hence, when $\sigma=1$ and $t_\nu=3$, $D(\varphi)$ becomes

$$D(\varphi)=\left\{\frac{c_1^{(0)}}{1-x_1}+\frac{c_1^{(1)}}{(1-x_1)^2}+\frac{c_1^{(2)}}{(1-x_1)^3}\right\}+\text{conj.}-B_0$$

which is the same as equation (6) in our preliminary report (Kakinoki & Komura, 1962).

With equations (77) and (79), equation (80) can be calculated for the three cases as follows:

In the case of different thickness:

$$c_\nu^{(n)}\to b_\nu^{(n)}=b_{\nu0}^{(n)}e^{i\rho_\nu{}^{(n)}},\ \varphi\to 0\ \text{and}\ x_\nu\to y_\nu=y_{\nu0}e^{i\delta_\nu}$$

$$B_m=\sum_{\nu=1}^{\sigma}B_m^{(\nu)},\quad B_m^{(\nu)}=\begin{cases}\sum_{n=0}^{m}{}_mC_ny_\nu^{m-n}b_\nu^{(n)} & \text{for } m\le t_\nu-2\\ \sum_{n=0}^{t_\nu-1}{}_mC_ny_\nu^{m-n}b_\nu^{(n)} & \text{for } m\ge t_\nu-1\end{cases}\tag{81}$$

$$D(\varphi)=\sum_{\nu=1}^{\sigma}\left\{b_{\nu0}^{(0)}\frac{(1-y_{\nu0}^2)\cos\varrho_\nu^{(0)}-2y_{\nu0}\sin\delta_\nu\sin\varrho_\nu^{(0)}}{1+y_{\nu0}^2-2y_{\nu0}\cos\delta_\nu}\right.$$
$$\left.+\sum_{n=1}^{t_\nu-1}2b_{\nu0}^{(n)}\frac{\sum_{s=0}^{1+n}(-1)^s{}_{1+n}C_sy_{\nu0}^s\cos(s\delta_\nu-\varrho_\nu^{(n)})}{(1+y_{\nu0}^2-2y_{\nu0}\cos\delta_\nu)^{1+n}}\right\}.\tag{82}$$

In the case of equal thickness:

$$c_\nu^{(n)}\to d_\nu^{(n)}=d_{\nu0}^{(n)}e^{i\rho_\nu{}^{(n)}},\quad\text{and}\quad x_\nu=x_{\nu0}e^{i\delta_\nu}$$

$$J_m=\sum_{\nu=1}^{\sigma}J_m^{(\nu)},\quad J_m^{(\nu)}=\begin{cases}\sum_{n=0}^{m}{}_mC_n\,x_\nu^{m-n}d_\nu^{(n)} & \text{for } m\le t_\nu-2\\ \sum_{n=0}^{t_\nu-1}{}_mC_n\,x_\nu^{m-n}d_\nu^{(n)} & \text{for } m\ge t_\nu-1\end{cases}\tag{83}$$

$$D(\varphi)=\sum_{\nu=1}^{\sigma}\left[d_{\nu0}^{(0)}\frac{(1-x_{\nu0}^2)\cos\varrho_\nu^{(0)}+2x_{\nu0}\sin(\varphi-\delta_\nu)\sin\varrho_\nu^{(0)}}{1+x_{\nu0}^2-2x_{\nu0}\cos(\varphi-\delta_\nu)}\right.$$
$$\left.+\sum_{n=1}^{t_\nu-1}2d_{\nu0}^{(n)}\frac{\sum_{s=0}^{1+n}(-1)^s{}_{1+n}C_s\,x_{\nu0}^s\cos\{(n-s)\varphi+s\delta_\nu-\varrho_\nu^{(n)}\}}{\{1+x_{\nu0}^2-2x_{\nu0}\cos(\varphi-\delta_\nu)\}^{1+n}}\right].\tag{84}$$

In the case of displacement stacking faults:

All corresponding equations with c (for d) and T (for J) to those given above. (85)

$\sum_{\nu=1}^{\sigma}D'_\nu(\varphi)$ in equation (80) can be arranged in a single form as follows:

Equation (73) is expanded with respect to x as

$$F(x)=\prod_{\nu=1}^{\sigma}(x-x_\nu)^{t_\nu}=\sum_{n=0}^{R}a_nx^{R-n}=0\tag{86}$$

and $f_\nu^{(q)}(x)$ is defined as

$$f_\nu^{(q)}(x)=\frac{F(x)}{(x-x_\nu)^q}=\sum_{s=0}^{R-q}b_s^{(\nu q)}\,x^{R-q-s}$$
$$=\sum_{s=0}^{R-q}\left(\sum_{m=0}^{s}{}_{s-m+q-1}C_{q-1}\,a_m\,x_\nu^{s-m}\right)x^{R-q-s}.\tag{87}$$

By the use of these relations, $\sum_{\nu=1}^{\sigma}D'_\nu(\varphi)$ can be transformed as follows:

$$\sum_{\nu=1}^{\sigma}D'_\nu(\varphi)=\sum_{\nu=1}^{\sigma}\sum_{n=0}^{t_\nu-1}\frac{c_\nu^{(n)}e^{i\varphi}}{(e^{i\varphi}-x_\nu)^{1+n}}$$
$$=\sum_{\nu=1}^{\sigma}\frac{e^{i\varphi}\sum_{n=0}^{t_\nu-1}c_\nu^{(n)}(e^{i\varphi}-x_\nu)^{t_\nu-n-1}}{(e^{i\varphi}-x_\nu)^{t_\nu}}$$
$$=\frac{e^{i\varphi}}{F(e^{i\varphi})}\sum_{\nu=1}^{\sigma}\sum_{n=0}^{t_\nu-1}c_\nu^{(n)}f_\nu^{(n+1)}(e^{i\varphi})$$
$$=\frac{e^{iR\varphi}}{F(e^{i\varphi})}\sum_{\nu=1}^{\sigma}\sum_{n=0}^{t_\nu-1}c_\nu^{(n)}\sum_{s=0}^{R-n-1}e^{-i(s+n)\varphi}\sum_{m=0}^{s}{}_{s-m+n}C_n\,a_m\,x_\nu^{s-m}$$
$$=\frac{e^{iR\varphi}}{F(e^{i\varphi})}\sum_{\nu=1}^{\sigma}\sum_{n=0}^{t_\nu-1}c_\nu^{(n)}\sum_{q=0}^{R-n-1}{}_{q+n}C_n\,x_\nu^q\sum_{m=0}^{R-1-n-q}a_me^{-i(m+n+q)\varphi}$$
$$=\frac{e^{iR\varphi}}{F(e^{i\varphi})}\sum_{\nu=1}^{\sigma}\left\{\sum_{r=0}^{t_\nu-2}\left(\sum_{m=0}^{R-1-r}a_me^{-i(m+r)\varphi}\right)\sum_{n=0}^{r}c_\nu^{(n)}{}_rC_n\,x_\nu^{r-n}\right.$$
$$\left.+\sum_{r=t_\nu-1}^{R-1}\left(\sum_{m=0}^{R-1-r}a_me^{-i(m+r)\varphi}\right)\sum_{n=0}^{t_\nu-1}c_\nu^{(n)}{}_rC_n\,x_\nu^{r-n}\right\}$$

$$= \frac{e^{iR\varphi}}{F(e^{i\varphi})} \sum_{r=0}^{R-1} \left(\sum_{m=0}^{R-1-r} a_m e^{-i(m+r)\varphi} \right) \sum_{\nu=1}^{\sigma} T_r^{(\nu)} .$$

$$\therefore \quad \sum_{\nu=1}^{\sigma} D'_\nu(\varphi) = \frac{\sum_{n=0}^{R-1} \left(\sum_{m=0}^{n} a_m T_{n-m} \right) e^{-in\varphi}}{\sum_{n=0}^{R} a_n e^{-in\varphi}} \quad (88)$$

which is equivalent to equations (35) and (45).

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Antiferromagnetism in nickel orthosilicate*.

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Nickel orthosilicate, Ni_2SiO_4, is isomorphous with the mineral olivine. Polycrystalline specimens were prepared from sodium orthosilicate and nickel nitrate. After the components were dissolved separately in distilled water, the orthosilicate solution was slowly added to the nitrate solution, yielding a hydrated nickel silicate precipitate. The precipitate was filtered and washed, and then fired at 1400 °C for 24 hours to give Ni_2SiO_4. Least-squares refinement of high-angle X-ray diffractometer data gave the lattice parameters $a = 10{\cdot}121 \pm 0{\cdot}005$, $b = 5{\cdot}915 \pm 0{\cdot}002$, $c = 4{\cdot}727 \pm 0{\cdot}002$ Å. The space group is *Pnma* with four formula-units per unit cell.

A vibrating-sample magnetometer was used to measure the magnetic susceptibility of Ni_2SiO_4. As shown in Fig. 1, the susceptibility follows a Curie–Weiss law above 60 °K, with $\Theta = 7$ °K and $p_{eff} = 3{\cdot}15\ \mu_B$. Kondo & Miyahara (1963) report slightly different values of -14 °K and $3{\cdot}04\ \mu_B$. The susceptibility goes through a maximum near 34 °K, indicative of a paramagnetic–antiferromagnetic transition.

Neutron diffraction patterns of polycrystalline Ni_2SiO_4 taken above and below the Néel temperature are shown in Fig. 2. The nuclear intensities (Table 1) agree well with values calculated from the olivine coordinates (Hanke & Zemann, 1963), confirming the crystal structure. The magnetic peaks in the low-temperature pattern cannot be in-

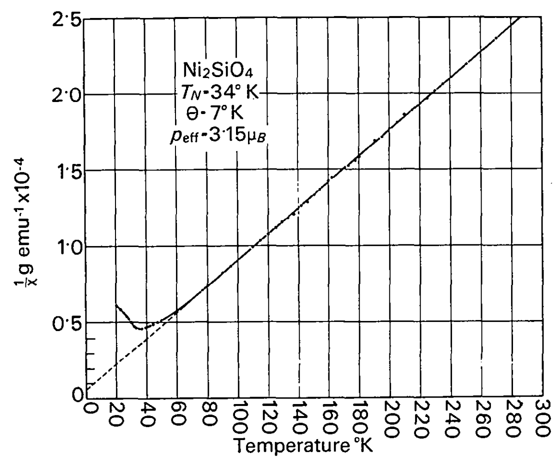

Fig. 1. The reciprocal susceptibility of Ni_2SiO_4 plotted as a function of temperature.

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