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Diffraction by a One-Dimensionally Disordered Crystal. II. Close-Packed Structures.

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Kakinoki & Komura's general theory on the intensity of X-ray diffuse scattering by one-dimensionally disordered crystals is applied to stacking faults occurring in close-packed structures. Practical examples are shown for the cases of s (Reichweite) = 1, 2, 3 and 4, which cover the results given by Paterson, Wilson and Jagodzinski. The cases of double (extrinsic)-deformation fault (Johnson), triple-deformation fault (Sato), multiple-deformation fault, single and double-deformation faults (Warren) and combinations of different kinds of faults are also dealt with by applying the general method without using difference equations.

Introduction

The general theory given in part I (Kakinoki & Komura, 1965) showed that the X-ray intensities of diffuse scattering from one-dimensionally disordered crystals can be calculated straightforwardly if a table of continuing probabilities for successive layers in each structure is correctly given. In this calculation, it is not necessary to follow a laborious procedure dealing with difference equations.

One of the important examples of one-dimensionally disordered crystals concerns displacement stacking faults, in particular the stacking faults occurring in cubic and hexagonal close-packed structures. The present paper shows the practical procedure for applying the general theory to these structures. The results so far obtained by many researchers are also discussed from the viewpoint of the new method.

General method of solution

In close-packed structures, there are three kinds of layer, A, B and C, for which the layer form factors can be expressed respectively as

$$V_A \equiv V_0,\ V_B = V_0\varepsilon^* \text{ and } V_C = V_0\varepsilon \quad \text{with } \varepsilon = \exp\{2\pi i(h-k)/3\}\,.$$

When $h-k=3n$ ($n=0, \pm 1, \pm 2, \ldots$), we have $\varepsilon=1$ and hence $V_A=V_B=V_C$. As a result, the well-known intensity formula

$$V_0V_0^* \sin^2(N\varphi/2)/\sin^2(\varphi/2)$$

is at once derived independently of the kind of fault. Here, N is the number of layers, and $\varphi=2\pi\zeta$, ζ being the continuous variable along a line parallel to $\mathbf{c}^*$; $\mathbf{c}^*$ is the axis reciprocal to $\mathbf{c}$ of the real crystal.

We treat hereafter only the cases in which $h-k=3n\pm 1$. Therefore, we have

$$\varepsilon=\exp(\pm i2\pi/3) = -\exp(\mp i\pi/3)$$
$$\varepsilon+\varepsilon^* = -1,\ \varepsilon^2=\varepsilon^*,\ \varepsilon^{*2}=\varepsilon \text{ and } \varepsilon^3=\varepsilon^{*3}=1$$

where the upper sign in $\pm$ or $\mp$ corresponds to the case $h-k=3n+1$ and the lower to the case $h-k=3n-1$. These two cases correspond to two kinds of line parallel to $\mathbf{c}^*$ in reciprocal space. For convenience, the line corresponding to $h-k=3n+1$ is called the *plus line* and that corresponding to $h-k=3n-1$ the *minus line*.

The intensity equation in the case of displacement stacking faults is given by equation (I-3)† *i.e.*

$$I_D(\varphi) = V_0V_0^*I(\varphi) = V_0V_0^*\{N + \sum_{m=1}^{N=1}(N-m)T_m e^{-im\varphi} + \text{conj.}\} \quad (1)$$

with

$$T_m = \text{spur } \boldsymbol{\varepsilon}\mathbf{F}\mathbf{P}^m \text{ and } T_0=1 \quad (2)$$

where conj. means the complex conjugate of the foregoing term and

$$(\boldsymbol{\varepsilon})_{ji} = \varepsilon_i\varepsilon_j^* \text{ and } (\mathbf{F})_{ij} = f_i\delta_{ij} \quad \therefore \quad (\boldsymbol{\varepsilon}\mathbf{F})_{ji} = f_i\varepsilon_i\varepsilon_j^*$$
$$(\mathbf{P})_{ij} = P_{ij}\,. \quad (3)$$

The parameter ε_i is the phase factor due to the displacement, parallel to the layer, of the origin of the layer i, and, in the present case,

$$\varepsilon_A=1,\ \varepsilon_B=\varepsilon^* \text{ and } \varepsilon_C=\varepsilon\,;$$

f_i is the existence probability of the layer i, and P_{ij} the continuing probability of the layer j to the layer i, δ_{ij} being Kronecker's delta.

Since a layer cannot follow a layer of the same kind in a close-packed structure, there are $R=3l$ ($l=2^{s-1}$) different configurations for s-layer sequences, where s is the *Reichweite* defined by Jagodzinski (1949*a*). We divide these R configurations into three groups, each consisting of l configurations, as follows (see Table 1). All l configurations from 1 to l belonging to the first group have an A layer at their terminal position. Similarly, those from $l+1$ to $2l$ belonging to the second

† (I-3) means equation (3) in part I (Kakinoki & Komura, 1965).

group have a B layer and those from $2l+1$ to $3l$ belonging to the third group a C layer. Thus the matrix $\boldsymbol{\varepsilon}$ can be expressed in the form

$$\boldsymbol{\varepsilon}=\begin{pmatrix}\mathbf{M} & \varepsilon^*\mathbf{M} & \varepsilon\mathbf{M}\\ \varepsilon\mathbf{M} & \mathbf{M} & \varepsilon^*\mathbf{M}\\ \varepsilon^*\mathbf{M} & \varepsilon\mathbf{M} & \mathbf{M}\end{pmatrix} \quad \text{with} \quad (\mathbf{M})_{ij}=1\,. \qquad (4)$$

The configuration $i+l$ $(i=1,2,\ldots,l)$ is obtained from the configuration i by the ABC cyclic change and the configuration $i+2l$ from the configuration $i+l$ by the ABC cyclic change. These three configurations, i, $i+l$ and $i+2l$, are said, for convenience, to belong to the *form i.* Some examples of the forms, with their notation, are shown in Table 1. Considering that the existence and continuing probabilities of configurations belonging to the same form should be the same, we can rewrite the matrices **F** and **P** as

$$\mathbf{F}=\tfrac{1}{3}\begin{pmatrix}\mathbf{W} & 0 & 0\\ 0 & \mathbf{W} & 0\\ 0 & 0 & \mathbf{W}\end{pmatrix} \quad \text{and} \quad \mathbf{P}=\begin{pmatrix}0 & \mathbf{P}_1 & \mathbf{P}_2\\ \mathbf{P}_2 & 0 & \mathbf{P}_1\\ \mathbf{P}_1 & \mathbf{P}_2 & 0\end{pmatrix}, \qquad (5)$$

where $(\mathbf{W})_{ij}=w_i\delta_{ij}$ and $w_i/3=f_i=f_{i+l}=f_{i+2l}$ $(i=1,2,\ldots,l)$. As a result, T_m in equation (2) can easily be reduced to

$$T_m=\operatorname{spur}\mathbf{H}(\varepsilon\mathbf{P}_1+\varepsilon^*\mathbf{P}_2)^m \text{ with } \mathbf{H}=\mathbf{MW} \qquad (6)$$

by mathematical induction, where the orders of the matrices **H**, **M**, **W**, $\mathbf{P}_1$ and $\mathbf{P}_2$ are all l. The relations spur $\mathbf{H}_0=1$ and $\mathbf{H}_0\mathbf{P}=\mathbf{H}_0$ in equation (I-12)† become

$$\operatorname{spur}\mathbf{H}=1 \text{ and } \mathbf{H}(\mathbf{P}_1+\mathbf{P}_2)=\mathbf{H}\,. \qquad (7)$$

Now that we can reduce the orders of the matrices to be used in the calculation, we may apply the general method of solution introduced in part I to the present calculation. The whole procedure for the calculation including the reduction is, after all, summarized in the form of the following five steps:

Step 1. Set $\mathbf{P}_1$ and $\mathbf{P}_2$ from the correct **P**.

Step 2. Express the existence probability, w_i, of the form i in terms of P_{ij} by solving equation (7).

Step 3. Calculate $T_0=1$, $T_1,\ldots,T_{l-1}$ by equation (6).

Step 4. Expand the characteristic equation $F(x)$ with respect to x

$$\left.\begin{aligned}F(x)&=\det(x\mathbf{1}-\varepsilon\mathbf{P}_1-\varepsilon^*\mathbf{P}_2)\\ &=\sum_{n=0}^{l} a_n x^{l-n}=0 \text{ with } a_0=1\end{aligned}\right\}. \qquad (8)$$

Step 5. Substitute T_m and a_n into

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

where

$$C_p=\sum_{n=0}^{l-p} a_n a^*_{n+p} \text{ and } D_p=\sum_{n=0}^{l-1-p} a_n E_{n+p}$$

with

$$E_q=\sum_{n=0}^{l} a^*_n T_{n-q}\ (q=1,2,\ldots,l-1)\ (T_{-m}=T^*_m)$$

$$E_0=\sum_{n=0}^{l-1} a^*_n T_n - a^*_l \sum_{n=1}^{l} a_n T_{l-n}\,.$$

Here, **1** is a unit matrix of the order l, and the characteristic equation $F(x)=0$ should be fulfilled for diagonalization of the matrix $(\varepsilon\mathbf{P}_1+\varepsilon^*\mathbf{P}_2)$. The intensity equation and the other quantities in step 5 are given by equation (I-46) and equations from (I-41*a*) to

† **H** in equation (I-12) is expressed here as $\mathbf{H}_0$ in order to avoid confusion with **H** in equation (6), the order of matrix being $3l$ for $\mathbf{H}_0$ and l for **H**.

Table 1. *Configurations of s-layer sequences belonging to the same form and their notation*

s	$l=2^{s-1}$	No. of form	$R=3l$	R configurations: 1st group from 1 to l	2nd group from $l+1$ to $2l$	3rd group from $2l+1$ to $3l$	Notation of the form	
2	2	1	6	*CA*	*AB*	*BC*	*S*	positive pair
		2		*BA*	*CB*	*AC*	*G*	negative pair
3	4	1	12	*BCA*	*CAB*	*ABC*	*c* = *SS*	positive cubic form
		2		*ACA*	*BAB*	*CBC*	*h* = *GS*	positive hexagonal form
		3		*ABA*	*BCB*	*CAC*	*h′* = *SG*	negative hexagonal form
		4		*CBA*	*ACB*	*BAC*	*c′* = *GG*	negative cubic form
4	8	1	24	*ABCA*	*BCAB*	*CABC*	*cc* = *SSS*	positive 4-layer form
		2		*CBCA*	*ACAB*	*BABC*	*hc* = *GSS*	positive 4-layer form
		3		*CACA*	*ABAB*	*BCBC*	*h′h* = *SGS*	positive 4-layer form
		4		*BACA*	*CBAB*	*ACBC*	*c′h* = *GGS*	positive 4-layer form
		5		*CABA*	*ABCB*	*BCAC*	*ch′* = *SSG*	negative 4-layer form
		6		*BABA*	*CBCB*	*ACAC*	*hh′* = *GSG*	negative 4-layer form
		7		*BCBA*	*CACB*	*ABAC*	*h′c′* = *SGG*	negative 4-layer form
		8		*ACBA*	*BACB*	*CBAC*	*c′c′* = *GGG*	negative 4-layer form

The terms *positive* and *negative* (Patterson & Kasper, 1959) are used according as the last pair is S or G.

(I-41d), with R and B_m replaced by l and T_m respectively. Explicit expressions of C_p, D_p, E_q and $D(\varphi)$ for $l=1$, 2, 3 and 4 are listed below, and are obtained from equations (I-42a)–(I-44b) with R and B_m replaced by l and T_m respectively.

Formula 1 ($l=1$)

$$D(\varphi)=\frac{1-a_1a_1^*}{1+a_1a_1^*+a_1^*\exp(i\varphi)+a_1\exp(-i\varphi)}\,.$$

Formula 2 ($l=2$)

$$C_0=1+a_1a_1^*+a_2a_2^*\quad C_1=a_1^*+a_1a_2^*\quad C_2=a_2^*$$
$$D_0=1+a_1a_1^*-a_2a_2^*+a_1^*T_1+a_1T_1^*\quad D_1=a_1^*+a_2^*T_1+T_1^*\,.$$

Formula 3 ($l=3$)

$$C_0=1+a_1a_1^*+a_2a_2^*+a_3a_3^*\quad C_1=a_1^*+a_1a_2^*+a_2a_3^*$$
$$C_2=a_2^*+a_1a_3^*\quad C_3=a_3^*$$
$$\begin{cases}E_0=1-a_3a_3^*+(a_1^*-a_2a_3^*)T_1+(a_2^*-a_1a_3^*)T_2\\ E_1=a_1^*+a_2^*T_1+T_1^*+a_3^*T_2\\ E_2=a_2^*+a_3^*T_1+a_1^*T_1^*+T_2^*\end{cases}$$
$$D_0=E_0+a_1E_1+a_2E_2\quad D_1=E_1+a_1E_2\quad D_2=E_2\,.$$

Formula 4 ($l=4$)

$$C_0=1+a_1a_1^*+a_2a_2^*+a_3a_3^*+a_4a_4^*$$
$$C_1=a_1^*+a_1a_2^*+a_2a_3^*+a_3a_4^*$$
$$C_2=a_2^*+a_1a_3^*+a_2a_4^*\quad C_3=a_3^*+a_1a_4^*\quad C_4=a_4^*$$
$$\begin{cases}E_0=1-a_4a_4^*+(a_1^*-a_3a_4^*)T_1+(a_2^*-a_2a_4^*)T_2\\ \qquad+(a_3^*-a_1a_4^*)T_3\\ E_1=a_1^*+a_2^*T_1+T_1^*+a_3^*T_2+a_4^*T_3\\ E_2=a_2^*+a_3^*T_1+a_1^*T_1^*+a_4^*T_2+T_2^*\\ E_3=a_3^*+a_4^*T_1+a_2^*T_1^*+a_1^*T_2^*+T_3^*\end{cases}$$
$$D_0=E_0+a_1E_1+a_2E_2+a_3E_3\quad D_1=E_1+a_1E_2+a_2E_3$$
$$D_2=E_2+a_1E_3\quad D_3=E_3\,.$$

Application to the cases of various values of the Reichweite *s*.

In this section, we show the practical procedure for obtaining the intensity equation and necessary quantities in the cases in which the Reichweite $s=1$, 2, 3 and 4. The results obtained by other researchers are also discussed.

(i) $s=1$ (*Paterson*)

The continuing table for $s=1$ is shown in Table 2. Such a table will be called hereafter a **P**-table or a complete **P**-table. Following the five steps and using formula 1 we obtain

Step 1: $\mathbf{P}_1=\alpha$ and $\mathbf{P}_2=1-\alpha$.

Step 2: $w=1\quad\therefore\quad f_A=f_B=f_C=\frac{1}{3}$.
$(w_S=\alpha$ and $w_G=1-\alpha)$. (9)

Step 3: $T_m=\{\alpha\varepsilon+(1-\alpha)\varepsilon^*\}^m$.

Step 4: $F(x)=x-\{\alpha\varepsilon+(1-\alpha)\varepsilon^*\}=0$
$\therefore\quad a_1=-\{\alpha\varepsilon+(1-\alpha)\varepsilon^*\}$.

Step 5 with formula 1:

$$D_\pm(\varphi)=\frac{3\alpha(1-\alpha)}{2-3\alpha(1-\alpha)-2\alpha\cos(\varphi\mp120°)-2(1-\alpha)\cos(\varphi\pm120°)}$$
$$=\frac{3\alpha(1-\alpha)}{2-3\alpha(1-\alpha)+\cos\varphi\pm\sqrt{3}(1-2\alpha)\sin\varphi}\,.\quad(10)$$

Here, $D_+(\varphi)$ is the intensity distribution of X-ray diffuse scattering along the plus line, and $D_-(\varphi)$ that along the minus line.

Equation (10) is the same as equation [7]† given by Paterson (1952). Regarding equation (9) and Tables 3 and 4, refer to the next two paragraphs.

(ii) $s=2$ (*including Wilson's case*)

The complete **P**-table for $s=2$ is shown in Table 5. There are $R=3\times2^{s-1}=6$ configurations. Three of them, *i.e.* CA, AB and BC, belong to form 1, *i.e.* the positive pair S as shown in Table 1, and the remaining three, *i.e.* BA, CB and AC, to the negative pair G. If, for example, AB (S) is followed by C with a probability α, we get ABC, of which the last two layers are BC (S). On the other hand, if AB is followed by A with a probability $1-\alpha$, we get ABA, of which the last

† The numbers of equations given by other authors are put in square brackets.

Table 2. **P**-*table for* $s=1$ (*Paterson*)

		A	B	C
$f_A=\frac{1}{3}$	A	0	α	$1-\alpha$
$f_B=\frac{1}{3}$	B	$1-\alpha$	0	α
$f_C=\frac{1}{3}$	C	α	$1-\alpha$	0

Table 3. $\mathbf{P}_{1,2}$-*table for* $s=1$

		S	G
$w_S=\alpha$	S	α	$1-\alpha$
$w_G=1-\alpha$	G	α	$1-\alpha$

Table 4. **p**-*tables for* $s=1$

		c	h'
$w_c=\alpha^2$	c	α	$1-\alpha$
$w_h=\alpha(1-\alpha)$	h	α	$1-\alpha$

		c'	h
$w_{c'}=(1-\alpha)^2$	c'	$1-\alpha$	α
$w_{h'}=\alpha(1-\alpha)$	h'	$1-\alpha$	α

two layers are BA (G). In this situation S may be said to be followed by S with a probability α and by G with a probability $1-\alpha$. In this way, the complete **P**-table (Table 5) can be simplified as Table 6, which corresponds to the sum of $\mathbf{P}_1$ and $\mathbf{P}_2$. Such a table will be called hereafter a $\mathbf{P}_{1,2}$-table or a simplified $\mathbf{P}_{1,2}$-table. Following the five steps and using formula 2, we obtain

Step 1: $\mathbf{P}_1=\begin{pmatrix}\alpha & 0\\ 1-\alpha' & 0\end{pmatrix}$ and $\mathbf{P}_2=\begin{pmatrix}0 & 1-\alpha\\ 0 & \alpha'\end{pmatrix}$.

Step 2: $\begin{pmatrix}w_S & w_G\\ w_S & w_G\end{pmatrix}\begin{pmatrix}\alpha & 1-\alpha\\ 1-\alpha' & \alpha'\end{pmatrix}=\begin{pmatrix}w_S & w_G\\ w_S & w_G\end{pmatrix}$

and $w_S+w_G=1$.

From these equations, we have in general

$$(1-\alpha)w_S=(1-\alpha')w_G \text{ and } w_S+w_G=1 . \quad (11)$$

Solving these equations, we have

$$w_S=(1-\alpha')/(2-\alpha-\alpha') \text{ and}$$
$$w_G=(1-\alpha)/(2-\alpha-\alpha') \quad (12)$$

except for the case $\alpha=\alpha'=1$, for which we may arbitrarily choose the ratio $w_S:w_G$.

Step 3: $T_m=\dfrac{1}{2-\alpha-\alpha'}\,\text{spur}\begin{pmatrix}1-\alpha' & 1-\alpha\\ 1-\alpha' & 1-\alpha\end{pmatrix}\times\begin{pmatrix}\alpha\varepsilon & (1-\alpha)\varepsilon^*\\ (1-\alpha')\varepsilon & \alpha'\varepsilon^*\end{pmatrix}^m$

$\therefore\quad T_1=-(1+\alpha\varepsilon^*+\alpha'\varepsilon)/(2-\alpha-\alpha')$.

Step 4: $F(x)=\begin{vmatrix}x-\alpha\varepsilon & -(1-\alpha)\varepsilon^*\\ -(1-\alpha')\varepsilon & x-\alpha'\varepsilon^*\end{vmatrix}=$

$x^2-(\alpha\varepsilon+\alpha'\varepsilon^*)x-1+\alpha+\alpha'=0$

$\therefore\quad a_1=-(\alpha\varepsilon+\alpha'\varepsilon^*)$ and $a_2=-(1-\alpha-\alpha')$.

Step 5 with formula 2:

$C_0=2(1-\alpha-\alpha'+\alpha^2+\alpha'^2)+\alpha\alpha'$
$C_1=\alpha+\alpha'+\alpha\alpha'+\alpha(2-\alpha)\varepsilon+\alpha'(2-\alpha')\varepsilon^*$
$C_2=-(1-\alpha-\alpha')$
$D_0=3(1-\alpha)(1-\alpha')(\alpha+\alpha')/(2-\alpha-\alpha')\quad D_1=0$

$$\therefore\quad D_\pm(\varphi)=\frac{3(1-\alpha)(1-\alpha')(\alpha+\alpha')/(2-\alpha-\alpha')}{\left(\begin{array}{l}2(1-\alpha-\alpha'+\alpha^2+\alpha'^2)+\alpha\alpha'+(\alpha+\alpha')^2\cos\varphi\\ -2(1-\alpha-\alpha')\cos 2\varphi\mp\sqrt{3}(\alpha-\alpha')(2-\alpha-\alpha')\sin\varphi\end{array}\right)} . \quad (13)$$

Table 5. **P**-*table for* $s=2$ (*including Wilson's case*)

A blank part means that the element is 0.

			(S) C–A	(G) B–A	(S) A–B	(G) C–B	(S) B–C	(G) A–C
$f_{CA}=w_S/3$	(S)	C–A			α			$1-\alpha$
$f_{BA}=w_G/3$	(G)	B–A			$1-\alpha'$			α'
$f_{AB}=w_S/3$	(S)	A–B		$1-\alpha$			α	
$f_{CB}=w_G/3$	(G)	C–B		α'			$1-\alpha'$	
$f_{BC}=w_S/3$	(S)	B–C	α			$1-\alpha$		
$f_{AC}=w_G/3$	(G)	A–C	$1-\alpha'$			α'		

Table 6. $\mathbf{P}_{1,2}$-*table for* $s=2$

		S	G
$w_S=(1-\alpha')/(2-\alpha-\alpha')$	S	α	$1-\alpha$
$w_G=(1-\alpha)/(2-\alpha-\alpha')$	G	$1-\alpha'$	α'

Table 7. **p**-*tables for* $s=2$

		c	h'
$w_c=\alpha w_S$	c	α	$1-\alpha$
$w_h=(1-\alpha')w_G$	h	α	$1-\alpha$

		c'	h
$w_{c'}=\alpha' w_G$	c'	α'	$1-\alpha'$
$w_{h'}=(1-\alpha)w_S$	h'	α'	$1-\alpha'$

When $\alpha'=1-\alpha$ is substituted into equation (13), we get equation (10) corresponding to the case of Paterson ($s=1$). In this case, equation (12) becomes equation (9) and Table 6 becomes Table 3. Table 3 means that the probability of the positive continuation is equal to α irrespective of the kind of the foregoing pair, S or G. The situation is the same for the negative continuation and hence the Reichweite s can be reduced from 2 to 1.

When $\alpha'=\alpha$, Table 6 becomes Table 8 and we have

$$\begin{aligned} w_S=w_G=\tfrac{1}{2} &\text{ for } \alpha=\alpha'\neq 1 \\ w_S+w_G=1 &\text{ for } \alpha=\alpha'=1 \end{aligned} \tag{14}$$

and

$$D_+(\varphi)=D_-(\varphi)= \frac{3\alpha(1-\alpha)}{4-8\alpha+5\alpha^2+4\alpha^2\cos\varphi-4(1-2\alpha)\cos^2\varphi}, \tag{15}$$

which is the same as equation [14] given by Wilson (1942)†.

Thus, the case $s=2$ includes the cases of Paterson and Wilson as special cases. Regarding Table 7, refer to the next paragraph.

Table 8. $\mathbf{P}_{1,2}$-*table for* $s=2$ *with* $\alpha=\alpha'$ (*Wilson*)

		S	G
$w_S=\frac{1}{2}$	S	α	$1-\alpha$
$w_G=\frac{1}{2}$	G	$1-\alpha$	α

(iii) $s=3$ (*including Jagodzinski's case*)

The complete **P**-table for $s=3$ is shown in Table 9 and the corresponding $\mathbf{P}_{1,2}$-table is given by Table 10. There are $R=3\times 2^{s-1}=12$ configurations and $l=2^{s-1}=4$ forms which are c, h, h' and c' as shown in Table 1. In the present case, Table 10 is conveniently rewritten as Table 11. We call them hereafter the **p**-tables or the 'convenient **p**-tables'. The **p**-tables are in fact very convenient for examining what kind of regular structures can be derived for a given s.

If we put $\beta=\alpha$ and $\beta'=\alpha'$ in Table 11, we get Table 7 ($s=2$) and further, if we put $\alpha'=1-\alpha$ in Table 7, we get Table 4 ($s=1$).

If, from Table 11, we define

$$\mathbf{p}_c=\begin{pmatrix}\alpha & 0\\ \beta & 0\end{pmatrix},\quad \mathbf{p}_h=\begin{pmatrix}0 & 1-\alpha\\ 0 & 1-\beta\end{pmatrix},$$
$$\mathbf{p}'_c=\begin{pmatrix}\alpha' & 0\\ \beta' & 0\end{pmatrix},\quad \mathbf{p}'_h=\begin{pmatrix}0 & 1-\alpha'\\ 0 & 1-\beta'\end{pmatrix} \tag{16}$$

$$\mathbf{h}=\begin{pmatrix}w_c & w_h\\ w_c & w_h\end{pmatrix}\quad\text{and}\quad \mathbf{h}'=\begin{pmatrix}w'_c & w'_h\\ w'_c & w'_h\end{pmatrix}, \tag{17}$$

then **H**, $\mathbf{P}_1$ and $\mathbf{P}_2$ are expressed as

$$\mathbf{H}=\begin{pmatrix}\mathbf{h}\,\mathbf{h}'\mathbf{u}\\ \mathbf{h}\,\mathbf{h}'\mathbf{u}\end{pmatrix},\quad \mathbf{P}_1=\begin{pmatrix}\mathbf{p}_c & 0\\ \mathbf{u}\mathbf{p}'_h & 0\end{pmatrix}\ \text{and}$$
$$\mathbf{P}_2=\begin{pmatrix}0 & \mathbf{p}'_h\mathbf{u}\\ 0 & \mathbf{u}\mathbf{p}'_c\mathbf{u}\end{pmatrix}\ \text{with}\ \mathbf{u}=\begin{pmatrix}0 & & & 1\\ & & 1 & \\ & \cdot^{\cdot^{\cdot}} & & \\ 1 & & & 0\end{pmatrix}_{l/2}. \tag{18}$$

Here, $\mathbf{p}_c$ and $\mathbf{p}'_c$ come from the left halves of **p**-tables and the suffix c means that the continuation is of cubic type. Similarly, $\mathbf{p}_h$ and $\mathbf{p}'_h$ come from the right halves of **p**-tables and the suffix h means that the continuation is of hexagonal type. Substitution of equation (18) into equations (6) and (7) gives

$$(6)\rightarrow T_m=\text{spur}\begin{pmatrix}\mathbf{h} & \mathbf{h}'\\ \mathbf{h} & \mathbf{h}'\end{pmatrix}\begin{pmatrix}\varepsilon\mathbf{p}_c & \varepsilon^*\mathbf{p}_h\\ \varepsilon\mathbf{p}'_h & \varepsilon^*\mathbf{p}'_c\end{pmatrix}^m \tag{19}$$

$$(7)\rightarrow \begin{cases}\mathbf{h}\mathbf{p}_c+\mathbf{h}'\mathbf{p}'_h=\mathbf{h}\\ \mathbf{h}'\mathbf{p}'_c+\mathbf{h}\mathbf{p}_h=\mathbf{h}'\end{cases}\ \text{and spur}(\mathbf{h}+\mathbf{h}')=1\,. \tag{20}$$

As a result, the characteristic equation (8) becomes

$$(8)\rightarrow F(x)=\begin{vmatrix}x\mathbf{1}-\varepsilon\mathbf{p}_c & -\varepsilon^*\mathbf{p}_h\\ -\varepsilon\mathbf{p}'_h & x\mathbf{1}-\varepsilon^*\mathbf{p}'_c\end{vmatrix}=0\,. \tag{21}$$

Now, the five steps are as follows:

Step 1: Equation (16).

Step 2: Equation (20). These matrix relations correspond to the simultaneous equations

$$\begin{cases} w_h=w'_h \qquad w_c+w'_c+2w_h=1\\ \beta w_h=(1-\alpha)w_c \text{ and } \beta' w_h=(1-\alpha')w'_c\,. \end{cases} \tag{22}$$

Solving these equations, we obtain

$$\begin{aligned} &w_h=w'_h=(1-\alpha)(1-\alpha')/C\\ &\qquad w_c=\beta(1-\alpha')/C\ \ w'_c=\beta'(1-\alpha)/C \end{aligned} \tag{23}$$

where

$$C=2(1-\alpha)(1-\alpha')+\beta(1-\alpha')+\beta'(1-\alpha)\,. \tag{24}$$

Step 3 with equation (19):

$$T_m=\frac{1}{C}\,\text{spur}$$
$$\begin{pmatrix} \beta(1-\alpha') & (1-\alpha)(1-\alpha') & \beta'(1-\alpha) & (1-\alpha)(1-\alpha')\\ \beta(1-\alpha') & (1-\alpha)(1-\alpha') & \beta'(1-\alpha) & (1-\alpha)(1-\alpha')\\ \beta(1-\alpha') & (1-\alpha)(1-\alpha') & \beta'(1-\alpha) & (1-\alpha)(1-\alpha')\\ \beta(1-\alpha') & (1-\alpha)(1-\alpha') & \beta'(1-\alpha) & (1-\alpha)(1-\alpha') \end{pmatrix}$$
$$\times\begin{pmatrix} \alpha\varepsilon & 0 & 0 & (1-\alpha)\varepsilon^*\\ \beta\varepsilon & 0 & 0 & (1-\beta)\varepsilon^*\\ 0 & (1-\alpha')\varepsilon & \alpha'\varepsilon^* & 0\\ 0 & (1-\beta')\varepsilon & \beta'\varepsilon^* & 0 \end{pmatrix}^m.$$

† Regarding the relation between the symbols used by Wilson and those used by the present author, refer to Kakinoki & Komura (1954*a*).

$$\therefore \quad T_1=-w_h+w_c\varepsilon+w_c'\varepsilon^* \quad T_2=T_1^*+3w_h$$
$$T_3=1-3(1-\beta\varepsilon-\beta'\varepsilon^*)w_h\,. \qquad (25)$$

Step 4 with equation (21):

$$F(x)=\begin{vmatrix} x-\alpha\varepsilon & 0 & 0 & -(1-\alpha)\varepsilon^* \\ -\beta\varepsilon & x & 0 & -(1-\beta)\varepsilon^* \\ 0 & -(1-\alpha')\varepsilon & x-\alpha'\varepsilon^* & 0 \\ 0 & -(1-\beta')\varepsilon & -\beta'\varepsilon^* & x \end{vmatrix}=0\,. \qquad (26)$$

$$\therefore \quad \begin{cases} a_1=-(\alpha\varepsilon+\alpha'\varepsilon^*) \quad a_2=\alpha\alpha'-(1-\beta)(1-\beta') \\ a_3=(1-\beta')(\alpha-\beta)\varepsilon+(1-\beta)(\alpha'-\beta')\varepsilon^* \\ a_4=-(\alpha-\beta)(\alpha'-\beta')\,. \end{cases} \qquad (27)$$

Step 5 with formula 4:

$$C_0=1+\alpha^2+\alpha'^2-\alpha\alpha'\{1-\alpha\alpha'+2(1-\beta)(1-\beta')\}$$
$$-(\alpha-\beta)(\alpha'-\beta')(1-\beta)(1-\beta')$$
$$+\{(1-\beta)^2+(\alpha-\beta)^2\}\{(1-\beta')^2+(\alpha'-\beta')^2\}$$

$$C_1=-(C_{11}\varepsilon+C_{12}\varepsilon^*)$$

$$\begin{cases} C_{11}=\alpha'(1+\alpha^2)-\alpha(1-\beta)\{1-\beta'+\alpha'(\alpha'-\beta')\} \\ \qquad +(\alpha'-\beta')(1-\beta')\{(1-\beta)^2+(\alpha-\beta)^2\} \\ C_{12}=(\text{exchange } ' \text{ in } C_{11}) \end{cases}$$

Table 9. **P**-*table for* $s=3$ (*including Jagodzinski's case*)

	c B	h A	h' A	c' C	c C	h B	h' B	c' A	c A	h C	h' C	c' B
c B					α						$1-\alpha$	
h A					β						$1-\beta$	
h' A						$1-\beta'$						β'
c' C						$1-\alpha'$						α'
c C			$1-\alpha$						α			
h B			$1-\beta$						β			
h' B				β'						$1-\beta'$		
c' A				α'						$1-\alpha'$		
c A	α						$1-\alpha$					
h C	β						$1-\beta$					
h' C		$1-\beta'$						β'				
c' B		$1-\alpha'$						α'				

Table 10. $\mathbf{P}_{1,2}$-*table for* $s=3$

	c	h	h'	c'
c	α		$1-\alpha$	
h	β		$1-\beta$	
h'		$1-\beta'$		β'
c'		$1-\alpha'$		α'

Table 11. **p**-*tables for* $s=3$

	c	h'
c	α	$1-\alpha$
h	β	$1-\beta$

	c'	h
c'	α'	$1-\alpha'$
h'	β'	$1-\beta'$

$$C_2 = C_{20} - (C_{21}\varepsilon + C_{22}\varepsilon^*)$$

$$\begin{cases} C_{20} = \{\alpha\alpha' - (1-\beta)(1-\beta')\}\{1-(\alpha-\beta)(\alpha'-\beta')\} \\ \qquad -\alpha(\alpha-\beta)(1-\beta') - \alpha'(\alpha'-\beta')(1-\beta) \\ C_{21} = \alpha'(\alpha-\beta)(1-\beta') \quad C_{22} = \alpha(\alpha'-\beta')(1-\beta) \end{cases}$$

$$C_3 = C_{31}\varepsilon + C_{32}\varepsilon^*$$

$$\begin{cases} C_{31} = (\alpha'-\beta')\{1-\beta+\alpha(\alpha-\beta)\} \\ C_{32} = (\alpha-\beta)\{1-\beta'+\alpha'(\alpha'-\beta')\} \end{cases}$$

$$C_4 = -(\alpha-\beta)(\alpha'-\beta') = -C_{40}$$

$$\begin{cases} E_0 = 3w_h[\beta'(1+\alpha'-\beta')\{1-\beta(\alpha-\beta) \\ \qquad -\alpha'(\alpha-\beta)\varepsilon\} \\ \qquad +\beta(1+\alpha-\beta)\{1-\beta'(\alpha'-\beta') \\ \qquad -\alpha(\alpha'-\beta')\varepsilon^*\}] \\ E_1 = -3w_h[\beta\beta' + \beta\{\alpha'+(\alpha-\beta)(\alpha'-\beta')\}\varepsilon \\ \qquad +\beta'\{\alpha+(\alpha-\beta)(\alpha'-\beta')\}\varepsilon^*] \\ E_2 = E_3 = 0 \end{cases}$$

$$D_0 = 3w_h[\beta(1+\alpha-\beta)\{1+(\alpha'-\beta')^2\} + \beta'(1+\alpha'-\beta')\{1+(\alpha-\beta)^2\}] \equiv 3w_h D'_o$$

$$D_1 = -3w_h(D_{11}\varepsilon + D_{12}\varepsilon^*)$$

$$\begin{cases} D_{11} = \beta(\alpha'-\beta')(1+\alpha-\beta) \\ D_{12} = \beta'(\alpha-\beta)(1+\alpha'-\beta') \end{cases}$$

$$D_2 = D_3 = 0$$

$$\therefore \quad D_\pm(\varphi) = X_\pm(\varphi)/Y_\pm(\varphi) \tag{28}$$

$$\begin{cases} X_\pm(\varphi) = 3w_h\{D'_0 + 2D_{11}\cos(\varphi \mp 60°) \\ \qquad + 2D_{12}\cos(\varphi \pm 60°)\} \qquad (28') \\ Y_\pm(\varphi) = C_0 + 2\{C_{11}\cos(\varphi \mp 60°) \\ \qquad + C_{12}\cos(\varphi \pm 60°) \\ \qquad + C_{20}\cos 2\varphi + C_{21}\cos(2\varphi \mp 60°) \\ \qquad + C_{22}\cos(2\varphi \pm 60°) \\ \qquad - C_{31}\cos(3\varphi \mp 60°) - C_{32}\cos(3\varphi \pm 60°) \\ \qquad - C_{40}\cos 4\varphi\}\,. \qquad (28'') \end{cases}$$

When $\beta'=0$, a factor $\{1+\alpha'^2+2\alpha'\cos(\varphi\mp 60°)\}$, which is the only factor including α', appears in both the numerator and the denominator of $D_\pm(\varphi)$. As a result, they are cancelled out, and this amounts to putting $\alpha'=0$. Thus we obtain

$$D_{\alpha\beta,\pm}(\varphi) = X_{\alpha\beta}/Y_{\alpha\beta,\pm}(\varphi) \tag{29}$$

$$\begin{cases} X_{\alpha\beta} = 3\beta(1-\alpha)(1+\alpha-\beta)/\{2(1-\alpha)+\beta\} \qquad (29') \\ Y_{\alpha\beta,\pm}(\varphi) = 2[1-\beta(1-\alpha)+(\alpha-\beta)^2 \\ \qquad + \{\alpha+(\alpha-\beta)(1-\beta)\}\cos(\varphi\pm 60°) \\ \qquad - \alpha(1-\beta)\cos(\varphi\mp 60°) \\ \qquad - \{1-\beta+\alpha(\alpha-\beta)\}\cos 2\varphi \\ \qquad - (\alpha-\beta)\cos(3\varphi\pm 60°)]\,. \qquad (29'') \end{cases}$$

In this case, since $\alpha'=\beta'=0$, then $C=2-2\alpha+\beta$ and we have

$$w'_c = 0,\ w_c = \beta/(2-2\alpha+\beta) \text{ and } w_h = w'_h = (1-\alpha)/(2-2\alpha+\beta)\,. \tag{30}$$

Therefore we may put

$$T_m = \frac{1}{2-2\alpha+\beta}\,\text{spur} \begin{pmatrix} \beta & (1-\alpha) & (1-\alpha) \\ \beta & (1-\alpha) & (1-\alpha) \\ \beta & (1-\alpha) & (1-\alpha) \end{pmatrix} \begin{pmatrix} \alpha\varepsilon & 0 & (1-\alpha)\varepsilon^* \\ \beta\varepsilon & 0 & (1-\beta)\varepsilon^* \\ 0 & \varepsilon & 0 \end{pmatrix}^m . \tag{31}$$

The same result as equation (29) can be obtained by applying steps 3, 4 and 5, with formula 3, direct to equation (31).

When $\beta=0$, the replacement

$$\alpha \to \alpha',\ \beta \to \beta',\ \pm \to \mp \text{ and } \mp \to \pm \tag{32}$$

can be made in the corresponding equations from (29) to (30).

In order to discuss the peak shift due to faults, as was found in practice in the case of β' martensite of Cu_3Al (Nishiyama, Kakinoki & Kajiwara, 1965; Kajiwara & Fujita, 1966 and Kajiwara, 1967), it is enough to study the derivative of $Y_{\alpha\beta,\pm}(\varphi)$ with respect to φ, because $X_{\alpha\beta}$ in equation (29) does not include φ.

If we put $\alpha'=\alpha$ and $\beta'=\beta$, we get

$$w_c = w'_c = \beta/\{2(1-\alpha+\beta)\} \text{ and } w_h = w'_h = (1-\alpha)/\{2(1-\alpha+\beta)\} \tag{33}$$

and the characteristic equation becomes

$$F(x) = x^4 + \alpha x^3 + \{\alpha^2-(1-\beta)^2\}x^2 - (1-\beta)(\alpha-\beta)x - (\alpha-\beta)^2 = 0\,. \tag{34}$$

Equation (34) is the same as the equation [10] given by Jagodzinski (1949*b*). The intensity equation then becomes

$$D_+(\varphi) = D_-(\varphi) = \frac{3\beta(1-\alpha)(1+\alpha-\beta)\{1+(\alpha-\beta)^2+(\alpha-\beta)\cos\varphi\}/(1-\alpha+\beta)}{\left(\begin{aligned} &2-4\beta-2\alpha\beta+7\beta^2+(\alpha-\beta)\{(\alpha-\beta)(2\alpha^2+3\beta^2)+2\beta(\alpha+3\beta)\} \\ &+2\{\alpha(2\beta+\alpha^2-\beta^2)+(\alpha-\beta)(1-\beta)(1-2\beta+2\beta^2-2\alpha\beta)\}\cos\varphi \\ &+2[\alpha^2-(1-\beta)^2-(\alpha-\beta)\{\alpha^2(\alpha-\beta)+\beta(1-\beta)(1+\alpha-\beta)\}]\cos 2\varphi \\ &-2(\alpha-\beta)(1-\beta+\alpha^2-\alpha\beta)\cos 3\varphi - 2(\alpha-\beta)^2\cos 4\varphi \end{aligned}\right)}\,. \tag{35}$$

Equation (35) becomes equation (15) (Wilson's case) when $\alpha=\beta$ ($s=2$).

(iv) $s\geq 4$ (*including Jagodzinski's case*)

We obtain Tables 2, 5 and 9 for larger values of s, and in the same way we can obtain the complete **P**-table for any value of s. However, such a complete **P**-table becomes larger, and hence the use of **p**-tables, with equations (18)–(21), is more convenient for larger s. We therefore show here only how the **p**-tables will change as s increases. The **p**-tables for $s=4$ are shown in Table 12.

The characteristic equation in this case is given as

$$F(x)=x^8+a_1x^7+a_2x^6+a_3x^5+a_4x^4+a_5x^3+a_6x^2+a_7x+a_8=0 \quad (36)$$

$$\begin{aligned}
a_1&=-(\alpha\varepsilon+\alpha'\varepsilon^*)\\
a_2&=\alpha\alpha'-(1-\gamma)(1-\gamma')\\
a_3&=\{\alpha(1-\gamma)(1-\gamma')-\gamma(1-\beta)(1-\delta')\}\varepsilon\\
&\quad+\{\alpha'(1-\gamma)(1-\gamma')-\gamma'(1-\beta')(1-\delta)\}\varepsilon^*\\
a_4&=-\alpha\alpha'(1-\gamma)(1-\gamma')-\delta\delta'(1-\beta)(1-\beta')\\
&\quad+\alpha\gamma'(1-\beta')(1-\delta)+\alpha'\gamma(1-\beta)(1-\delta')\\
&\quad+\gamma'(\alpha'-\beta')(1-\delta)\varepsilon+\gamma(\alpha-\beta)(1-\delta')\varepsilon^* \qquad (36')\\
a_5&=(\alpha-\beta)\{\delta\delta'(1-\beta')-\alpha'\gamma(1-\delta')\}\varepsilon\\
&\quad+(\alpha'-\beta')\{\delta\delta'(1-\beta)-\alpha\gamma'(1-\delta)\}\varepsilon^*\\
a_6&=(1-\beta)(1-\beta')(\gamma-\delta)(\gamma'-\delta')-\delta\delta'(\alpha-\beta)(\alpha'-\beta')\\
a_7&=-(\gamma-\delta)(\gamma'-\delta')\{(\alpha-\beta)(1-\beta')\varepsilon\\
&\quad+(\alpha'-\beta')(1-\beta)\varepsilon^*\}\\
a_8&=(\alpha-\beta)(\alpha'-\beta')(\gamma-\delta)(\gamma'-\delta')\,.
\end{aligned}$$

When all the primes are omitted, equation (36) is the same as the characteristic equation [36] given by Jagodzinski (1954).

Discussion

In the method mentioned above, the characteristic equation, $F(x)=0$, has l roots because the order of the matrices $\mathbf{P}_1$ and $\mathbf{P}_2$ is l. Hence we have at most l maxima on the calculated intensity curve. Let M be the number of the observed peaks within a period in reciprocal space corresponding to one layer thickness. Then we have the relation

$$M\leq l=2^{s-1}\,, \qquad (37)$$

which gives the minimum value of s to be considered.

If the characteristic equation has a root $|x_\nu|=1$, a Laue function of a form such as

$$c_\nu\,\frac{\sin^2\{N(\varphi-\delta_\nu)/2\}}{\sin^2\{(\varphi-\delta_\nu)/2\}} \qquad (38)$$

must be added to $ND_\pm(\varphi)$, where

$$c_\nu=\frac{\sum_{m=0}^{l-1}\left(\sum_{n=0}^{l-1-m}a_nT_{l-1-m-n}\right)x_\nu^m}{\sum_{n=0}^{l-1}(l-n)a_nx_\nu^{l-1-n}}$$

$$\text{and}\quad x_\nu=\exp(i\delta_\nu). \qquad (39)$$

In this case, a factor $\{1-\cos(\varphi-\delta_\nu)\}$ appears in both the numerator and the denominator of $D_\pm(\varphi)$ and they are cancelled out.

Substitution of equations (4) and (5) into equation (2) gives

$$T_m=\tfrac{1}{3}\,\mathrm{spur}\begin{pmatrix}\mathbf{H} & \varepsilon^*\mathbf{H} & \varepsilon\mathbf{H}\\ \varepsilon\mathbf{H} & \mathbf{H} & \varepsilon^*\mathbf{H}\\ \varepsilon^*\mathbf{H} & \varepsilon\mathbf{H} & \mathbf{H}\end{pmatrix}\begin{pmatrix}0 & \mathbf{P}_1 & \mathbf{P}_2\\ \mathbf{P}_2 & 0 & \mathbf{P}_1\\ \mathbf{P}_1 & \mathbf{P}_2 & 0\end{pmatrix}^m . \qquad (40)$$

Since, as is readily proved by mathematical induction, $\mathbf{P}^m$ takes the form

$$\mathbf{P}^m=\begin{pmatrix}\mathbf{X}_m & \mathbf{Y}_m & \mathbf{Y}'_m\\ \mathbf{Y}'_m & \mathbf{X}_m & \mathbf{Y}_m\\ \mathbf{Y}_m & \mathbf{Y}'_m & \mathbf{X}_m\end{pmatrix},$$

equation (40) becomes

$$T_m=P^0_m+\varepsilon P^+_m+\varepsilon^*P^-_m \qquad (41)$$

where

$$P^0_m=\mathrm{spur}\,\mathbf{HX}_m,\ P^+_m=\mathrm{spur}\,\mathbf{HY}_m\ \text{and}\ P^-_m=\mathrm{spur}\,\mathbf{HY}'_m\,. \qquad (42)$$

Here, P^0_m, P^+_m and P^-_m are respectively interpreted as the probabilities of finding the layer m to be the same as, one ahead of, and one behind the zero layer, in the ABC sequence. Using equation (41), we can express $D_+(\varphi)$ and $D_-(\varphi)$ as

$$D_+(\varphi)=\sum_{m=-\infty}^{\infty}T^+_me^{-im\varphi}\ \text{and}$$

$$D_-(\varphi)=\sum_{m=-\infty}^{\infty}T^{+*}_me^{-im\varphi} \qquad (43)$$

where

$$T^\pm_{-m}=T^{+*}_m\ \text{and}\ T^+_m=P^0_m+\varepsilon_0P^+_m+\varepsilon^*_0P^-_m \qquad (44)$$

with

$$\varepsilon_0=\exp(2\pi i/3)=(-1+\sqrt{3}i)/2\,.$$

From equation (43), we find that the relation

$$D_+(-\varphi)=D_-(\varphi) \qquad (45)$$

Table 12. **p**-*tables for* $s=4$ (*including Jagodzinski's case*)

	cc	hc	hh'	ch'
cc	α			$1-\alpha$
hc	β			$1-\beta$
$h'h$		γ	$1-\gamma$	
$c'h$		δ	$1-\delta$	

	$c'c'$	$h'c'$	$h'h$	$c'h$
$c'c'$	α'			$1-\alpha'$
$h'c'$	β'			$1-\beta'$
hh'		γ'	$1-\gamma'$	
ch'		δ'	$1-\delta'$	

holds in general. This equation means that the intensity distributions along the plus line and the minus line are mutually antisymmetric with respect to the points $\varphi = n\pi$. This is the case for equations (10), (13) and (28).

On the other hand, when the condition

$$P_m^+ = P_m^- = (1 - P_m^0)/2 \ (P_m^0 + P_m^+ + P_m^- = 1) \quad (46)$$

is satisfied, the relation

$$D_+(\varphi) = D_-(\varphi) = D_+(-\varphi) = D_-(-\varphi) = \sum_{m=-\infty}^{\infty} (\tfrac{3}{2}P_m^0 - \tfrac{1}{2}) e^{-im\varphi} = \sum_{m=-\infty}^{\infty} (\tfrac{3}{2}P_m^0 - \tfrac{1}{2}) \cos m\varphi \quad (47)$$

holds. This means that the intensity distributions along the plus line and the minus line are not only the same but also symmetric with respect to the points $\varphi = n\pi$ on each line. This is the case for equation (15) (Wilson) and (35) (Jagodzinski). In deriving these equations, we omitted all primes in Tables 5 and 9, and this omission leads to the result

$$\mathbf{P}_2 = \mathbf{U}\mathbf{P}_1\mathbf{U} \text{ with } \mathbf{U} = \begin{pmatrix} 0 & & & 1 \\ & & 1 & \\ & \cdot^{\cdot^{\cdot}} & & \\ 1 & & & 0 \end{pmatrix}_l . \quad (48)$$

Equation (48) means that $\mathbf{P}_2$ is obtained from $\mathbf{P}_1$ by inversion with respect to the centre of the matrix. In this case, we can show that

$$\mathbf{Y}'_m = \mathbf{U}\mathbf{Y}_m\mathbf{U} \quad (49)$$

by mathematical induction (Kakinoki & Komura, 1954*a*). Consequently, from equation (42) we can see that the equality (47) holds because the condition (46) has been satisfied.

In order to analyse the mutually antisymmetric intensity distributions along the plus line and the minus line, we must distinguish quantities for a positive form, such as $w_i, \alpha, \beta, \ldots$ from those for the corresponding negative form, such as $w'_i, \alpha', \beta', \ldots$ (Kakinoki & Komura, 1954*b*). In fact, only by doing so could we analyse the pattern of β' martensite of Cu_3Al by the use of equation (28) (Nishiyama, Kakinoki & Kajiwara, 1965; Kajiwara & Fujita, 1966; Kajiwara, 1967).

There have been published a number of calculations for various models such as double (extrinsic)-deformation fault (Johnson, 1963), triple-deformation fault (Sato, 1966), single- and double-deformation faults (Warren, 1963), deformation and twin (growth) faults (Gevers, 1954; Warren, 1959). Although all these cases have so far been treated by the difference equation method, they can be treated more easily and less ambiguously by the present method if the **P**-table is correctly set in each case as shown in the Appendix, except for the case of deformation and twin (growth) faults treated by Gevers and Warren, which involves some problems to be further discussed elsewhere.

APPENDIX

Calculations for various models proposed by other investigators and for related models

Many calculations by the difference equation method, based on various models, have been reported. Here we show that the same results can be derived more easily and less ambiguously by the present method. In order to save the space, we show only important points of calculation without any detailed explanation.

(1) *Double (extrinsic)-deformation fault (Johnson, 1963)*

The complete **P**-table is shown in Table 13 and we have

Step 1: $\mathbf{P}_1 = \begin{pmatrix} 1-\alpha' & 0 \\ 0 & 0 \end{pmatrix}$ and $\mathbf{P}_2 = \begin{pmatrix} 0 & \alpha' \\ 1 & 0 \end{pmatrix}$.

Step 2: $w = 1/(1+\alpha')$ and $w' = \alpha'/(1+\alpha')$.

Step 3: $T_m = \dfrac{1}{1+\alpha'} \text{ spur} \begin{pmatrix} 1 & \alpha' \\ 1 & \alpha' \end{pmatrix} \begin{pmatrix} (1-\alpha')\varepsilon & \alpha'\varepsilon^* \\ \varepsilon^* & 0 \end{pmatrix}^m$

$\therefore \quad T_1 = \{-2\alpha' + (1-3\alpha')\varepsilon\}/(1+\alpha')$.

Step 4: $F(x) = \begin{vmatrix} x-(1-\alpha')\varepsilon & -\alpha'\varepsilon^* \\ -\varepsilon^* & x \end{vmatrix} = x^2 - (1-\alpha')\varepsilon x - \alpha'\varepsilon = 0$

$\therefore \quad a_1 = -(1-\alpha')\varepsilon$ and $a_2 = -\alpha'\varepsilon$.

Step 5 with formula 2:

$C_0 = 2(1-\alpha'+\alpha'^2)$ $C_1 = (1-\alpha')(\alpha'-\varepsilon^*)$ $C_2 = -\alpha'\varepsilon^*$

$D_0 = 6\alpha'(1-\alpha')/(1+\alpha')$ $D_1 = \{3\alpha'(1-\alpha')/(1+\alpha')\}\varepsilon$

$$D_\pm(\varphi) = \frac{3\alpha'(1-\alpha')}{1+\alpha'} \cdot \frac{1-\cos(\varphi \mp 60°)}{1-\alpha'+\alpha'^2+(1-\alpha')\{\alpha' \cos\varphi + \cos(\varphi \pm 60°)\} + \alpha' \cos(2\varphi \pm 60°)} . \quad (50)$$

Table 13. *Complete* **P**-*table for the case of double (extrinsic)-deformation fault (Johnson)*

		A	A'	B	B'	C	C'
$f_A = w/3 = 1/\{3(1+\alpha')\}$	A			$1-\alpha'$			α'
$f_{A'} = w'/3 = \alpha'/\{3(1+\alpha')\}$	A'					1	
$f_B = w/3$	B		α'			$1-\alpha'$	
$f_{B'} = w'/3$	B'	1					
$f_C = w/3$	C	$1-\alpha'$			α'		
$f_{C'} = w'/3$	C'			1			

Equation (50) is the same as equation [37] given by Johnson.

(2) *Triple-deformation fault* (*Sato*, 1966)

The complete **P**-table is shown in Table 14 and we have

Step 2: $w=1/(1+2\alpha'')$ and $w'=w''=\alpha''/(1+2\alpha'')$.

Step 3: $$T_m=\frac{1}{1+2\alpha''}\,\mathrm{spur}\begin{pmatrix}1 & \alpha'' & \alpha''\\ 1 & \alpha'' & \alpha''\\ 1 & \alpha'' & \alpha''\end{pmatrix}\begin{pmatrix}(1-\alpha'')\varepsilon & \alpha''\varepsilon^* & 0\\ 0 & 0 & \varepsilon^*\\ \varepsilon^* & 0 & 0\end{pmatrix}^m$$

$\therefore\quad T_1=\{(1-\alpha'')\varepsilon+3\alpha''\varepsilon^*\}/(1+2\alpha'')$ and
$T_2=\{-3\alpha''^2+(1-4\alpha'')\varepsilon^*\}/(1+2\alpha'')$.

Step 4: $$F(x)=\begin{vmatrix}x-(1-\alpha'')\varepsilon & -\alpha''\varepsilon^* & 0\\ 0 & x & -\varepsilon^*\\ -\varepsilon^* & 0 & x\end{vmatrix}=x^3-(1-\alpha'')\varepsilon x^2-\alpha''=0$$

$\therefore\quad a_1=-(1-\alpha'')\varepsilon\quad a_2=0$ and $a_3=-\alpha''$.

Step 5 with formula 3:

$C_0=2(1-\alpha''+\alpha''^2)$ $C_1=-(1-\alpha'')\varepsilon^*$
$C_2=\alpha''(1-\alpha'')\varepsilon$ $C_3=-\alpha''$

$E_0=\{1+2\alpha''-(1-\alpha''^2)\varepsilon\}E'$ $E_1=(-\alpha''+\varepsilon-\varepsilon^*)E'$
$E_2=\varepsilon^*E'$ with $E'=3\alpha''(1-\alpha'')/(1+2\alpha'')$

$D_0=3E'$ $D_1=2\varepsilon E'$ and $D_2=\varepsilon^*E'$

$$\therefore\quad D_\pm(\varphi)=\frac{6\alpha''(1-\alpha'')}{1+2\alpha''}\,\frac{1-\cos\varphi}{1-2\alpha''(1-\alpha'')-2\alpha''(1+\alpha'')\cos(\varphi\pm60^\circ)+4\alpha''\cos^2(\varphi\pm60^\circ)}\,. \qquad (51)$$

Equation (51) is the same as that given by Sato. In the present case, one of roots of the characteristic equation is $x_1=\varepsilon=\exp(\pm i120^\circ)$ and, from equation (39) we have $c_1=(1-f)^2$ where $f=3w'=3\alpha''/(1+2\alpha'')$. Hence we must add the Laue function

$$L_S(\varphi)=(1-f)^2\,\frac{\sin^2\{N(\varphi\mp120^\circ)/2\}}{\sin^2\{(\varphi\mp120^\circ)/2\}}$$

to $ND_\pm(\varphi)$. In the present case, the factor $\{1-\cos(\varphi\mp120^\circ)\}$ appears in both the numerator and the denominator of $D_\pm(\varphi)$ and they are cancelled out.

(3) *Multiple-deformation fault*

The calculation mentioned above can easily be extended to a more general case. We show here only $\mathbf{P}_1$ and $\mathbf{P}_2$ for $g=4$ and 5 where g is the number of the successive deformation faults.

$$g=4\ \mathbf{P}_1=\begin{pmatrix}1-\alpha & 0 & 0 & 0\\ 0 & 0 & 0 & 0\\ 0 & 0 & 0 & 0\\ 0 & 0 & 0 & 0\end{pmatrix}\quad \mathbf{P}_2=\begin{pmatrix}0 & \alpha & 0 & 0\\ 0 & 0 & 1 & 0\\ 0 & 0 & 0 & 1\\ 1 & 0 & 0 & 0\end{pmatrix}$$

$$g=5\ \mathbf{P}_1=\begin{pmatrix}1-\alpha & 0 & 0 & 0 & 0\\ 0 & 0 & 0 & 0 & 0\\ 0 & 0 & 0 & 0 & 0\\ 0 & 0 & 0 & 0 & 0\\ 0 & 0 & 0 & 0 & 0\end{pmatrix}\quad \mathbf{P}_2=\begin{pmatrix}0 & \alpha & 0 & 0 & 0\\ 0 & 0 & 1 & 0 & 0\\ 0 & 0 & 0 & 1 & 0\\ 0 & 0 & 0 & 0 & 1\\ 1 & 0 & 0 & 0 & 0\end{pmatrix}.$$

It is noticed that there is such a root as $|x_\nu|=1$ when $g=3n$.

(4) *Single and double-deformation faults* (*Warren*, 1963)

The complete **P**-table is shown in Table 15 and we have

Step 2: $w=1/(1+\alpha')$ and $w'=\alpha'/(1+\alpha')$.

Step 3: $$T_m=\frac{1}{1+\alpha'}\,\mathrm{spur}\begin{pmatrix}1 & \alpha'\\ 1 & \alpha'\end{pmatrix}\begin{pmatrix}(1-\alpha-\alpha')\varepsilon+\alpha\varepsilon^* & \alpha'\varepsilon^*\\ \varepsilon^* & 0\end{pmatrix}^m$$

$\therefore\quad T_1=-\{(\alpha+2\alpha')-(1-2\alpha-3\alpha')\varepsilon\}/(1+\alpha')$.

Step 4: $$F(x)=\begin{vmatrix}x-(1-\alpha-\alpha')\varepsilon-\alpha\varepsilon^* & -\alpha'\varepsilon^*\\ -\varepsilon^* & x\end{vmatrix}=x^2-\{(1-\alpha-\alpha')\varepsilon+\alpha\varepsilon^*\}x-\alpha'\varepsilon=0$$

$\therefore\quad a_1=-\{(1-\alpha-\alpha')\varepsilon+\alpha\varepsilon^*\}$ and $a_2=-\alpha'\varepsilon$.

Step 5 with formula 2:

$C_0=2(1-\alpha'+\alpha'^2)-3\alpha(1-\alpha-\alpha')$
$C_1=\alpha'(1-\alpha-\alpha')+\alpha(1-\alpha')$
$-\{(1-\alpha-\alpha')-\alpha(1-\alpha')\}\varepsilon^*$ $C_2=-\alpha'\varepsilon^*$
$D_0=\{2\alpha'+\alpha(1-\alpha')\}D'$ $D_1=\alpha'\varepsilon D'$ with
$D'=3(1-\alpha-\alpha')/(1+\alpha')$

Table 14. *Complete* **P**-*table for the case of triple-deformation fault* (*Sato*)

		A	A'	A''	B	B'	B''	C	C'	C''
$f_A=w/3=1/\{3(1+2\alpha'')\}$	A				$1-\alpha''$				α''	
$f_{A'}=w'/3=\alpha''/\{3(1+2\alpha'')\}$	A'									1
$f_{A''}=w''/3=\alpha''/\{3(1+2\alpha'')\}$	A''							1		
$f_B=w/3$	B		α''					$1-\alpha''$		
$f_{B'}=w'/3$	B'			1						
$f_{B''}=w''/3$	B''	1								
$f_C=w/3$	C	$1-\alpha''$				α''				
$f_{C'}=w'/3$	C'						1			
$f_{C''}=w''/3$	C''				1					

Table 15. *Complete* **P**-*table for the case of single- and double-deformation faults* (*Warren*)

		A	A'	B	B'	C	C'
$f_A=w/3=1/\{3(1+\alpha')\}$	A			$1-\alpha-\alpha'$		α	α'
$f_{A'}=w'/3=\alpha'/\{3(1+\alpha')\}$	A'					1	
$f_B=w/3$	B	α	α'			$1-\alpha-\alpha'$	
$f_{B'}=w'/3$	B'	1					
$f_C=w/3$	C	$1-\alpha-\alpha'$		α	α'		
$f_{C'}=w'/3$	C'			1			

Table 16. *A part of the complete* **P**-*table for the case of single-, double- and triple-deformation faults*

	(A)	B	B'	B''	B'''	C	C'	C''	C'''
A		$1-\alpha-\alpha'-\alpha''$				α	α'	α''	
A'						1			
A''									1
A'''						1			

$$D_\pm(\varphi)=\frac{3(1-\alpha-\alpha')}{1+\alpha'}\cdot\frac{2\alpha'+\alpha(1-\alpha')+2\alpha'\cos(\varphi\pm120^\circ)}{\left(\begin{array}{c}2(1-\alpha'+\alpha'^2)-3\alpha(1-\alpha-\alpha')+2\{\alpha'(1-\alpha-\alpha')+\alpha(1-\alpha')\}\cos\varphi\\ -2\{1-\alpha-\alpha'-\alpha(1-\alpha')\}\cos(\varphi\mp120^\circ)-2\alpha'\cos(2\varphi\mp120^\circ)\end{array}\right)}\,. \quad (52)$$

Equation (52) is easily verified to be the same as Warren's result. This equation becomes equation (50) (Johnson) for $\alpha=0$ and also equation (10) (Paterson) if α' is put equal to 0 and α is replaced by $1-\alpha$.

(5) *Combination of different kinds of faults*

Table 16 shows a part of the **P**-table in the case where single-, double- and triple-deformation faults coexist.

Table 17 shows the $\mathbf{P}_{1,2}$-table in the case where the case $s=2$, and single- and double-deformation faults coexist. We can similarly treat any combination of different kinds of fault when desired.

Table 17. $\mathbf{P}_{1,2}$-*table for the case where* $s=2$, *and single- and double-deformation faults coexist*

	S	G	G'
S	$1-\alpha-\alpha'$	α	α'
G	$1-\beta-\beta'$	β	β'
G'		1	

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