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The Diffraction of X-rays by Close-Packed Polytypic Crystals Containing Single Stacking Faults. I. General Theory

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Abstract

A general theory of X-ray diffraction by one-dimensionally disordered close-packed polytypic crystals has been developed. A random distribution of all possible single stacking faults for arbitrary n-periodical structure is taken into consideration. Exact expressions for measurable parameters of changes in the intensity distribution caused by faults are given. Initial equations of the theory have been formulated by applying Holloway's [*J. Appl. Phys.* (1969), **40**, 4313-4321] method of analytic solution. For the mathematical description of disorder, successive layers of the perfect structure have been denoted by an additional subscript j. The probability of occurrence of the faulted layer with subscript k after the layer with subscript j has been denoted by α_{jk}. A set of recurrence relations is developed for average phase factors of layers with subscript j on m positions. An arbitrary sequence of layers is written in these relations by using the so-called phase-change factors (after layer with subscript j), determined by Hägg's structure symbols. Terms of the coefficients of the characteristic equation and boundary conditions which are necessary to describe the change in the intensity distribution are given for small values of α_{jk}. Finally, the shifts and broadenings of the reciprocal-lattice points and the changes in the intensity of peak maxima are derived in terms of α_{jk}.

1. Introduction

Crystals exhibiting the phenomenon of polytypism also have a strong tendency for the formation of stacking faults. One-dimensionally disordered polytypic structures are often observed. This was found, among others, by Mitchell (1956), Jain & Trigunayat (1970), Lal & Trigunayat (1971), Minagawa (1977, 1978) and Pałosz (1981) in CdI_2 crystals, Jagodzinski (1954, 1971), Jagodzinski & Arnold (1960), Krishna & Marshall (1971*a*, *b*), Pandey & Krishna (1977) and Pandey, Lele & Krishna (1977) in SiC crystals, Prasad & Srivastava (1973), Minagawa (1975, 1979) and Chand & Trigunayat (1977) in PbI_2 crystals, Prager (1977) in AgI crystals, Mehrotra (1978) in CdBr crystals, Rai & Krishna (1968), Steinberger, Kiflawi, Kalman & Mardix (1973) and Farkas-Jahnke (1973*b*) in ZnS crystals, Iijima (1982) in mcGillite crystals, Kozielski (1975) and Pałosz & Przedmojski (1976*a*, *b*) in $Zn_{1-x}Cd_x$ and $ZnS_{1-x}Se_x$ mixed crystals, Demianiuk, Kaczmarek, Michalski & Zhmija (1979) and Michalski, Demianiuk, Kaczmarek & Zhmija (1979, 1981*a*, *b*, 1982) in different doped ZnS and ZnSe crystals and in $ZnS_{1-x}Se_x$ mixed crystals.

It is known that stacking faults involve changes in the intensity distribution of X-rays diffracted from the crystals. This phenomenon can be used for the characterization of the structured faultiness of crystals. For this purpose it is necessary to know the relationship between the measurable parameters of the changes in the intensity distribution and the parameters of structured faultiness.

The theory of X-ray diffraction by close-packed crystals with stacking faults was developed, among others, by Wilson (1942), Hendricks & Teller (1942), Jagodzinski (1949*a*, *b*), Paterson (1952), Gevers (1954), Johnson (1963), Allegra (1961, 1964), Kakinoki & Komura (1965), Kakinoki (1967), Howard (1977) and Frey & Boysen (1981). A satisfactory solution has been obtained for simple cases of X-ray diffraction by $3C$ and $2H$ crystals with stacking faults. Different models of $3C$ and $2H$ crystals containing growth faults, single (intrinsic)-, double (extrinsic)-, triple- and multiple-deformation faults have been considered.

The situation has been less satisfactory for the polytypic crystals. It is clear that more stacking faults can occur in the polytypic structures than in the most common $3C$ and $2H$ polymorphic modifications. Thus X-ray diffraction from polytypic crystals with stacking faults is also more difficult to describe. Gevers (1954) developed the theory only for $4H$ and $6H(33)$ crystals containing deformation faults. More general methods formulated by Hendricks & Teller (1942) and developed by Kakinoki & Komura (1965), Kakinoki (1967), Takaki & Sakurai (1976) and Takaki (1977) are quite complicated and they have not been widely used for polytypic structures. Minagawa (1977, 1978) used these methods to study the structural changes from $2H$ to $4H$ in CdI_2 crystals and the stacking faults in CdI_2-$4H$ crystals.

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At the same time, methods omitting the expression of X-ray intensity distribution by parameters of faultiness were developed, for example, in the works of Farkas-Jahnke (1973*a*, *b*), the method of model analysis of Pałosz (1977) and the method of optical models of Gauthier & Michel (1977). However, calculations were always too complicated and information about the structure was in some cases insufficient because of ambiguities which are admissible in these methods.

None of the methods seems to be applicable for the complete characterization of the structural faultiness in the general case of polytypic crystals. The first complete expression for the X-ray intensity distribution in reciprocal space for the simplest polytypic structure $4H$ with stacking faults was derived by Prasad & Lele (1971). All seven types of intrinsic faults in the $4H$ structure were taken into account in this theory. The average phase factor $\langle \exp[i\varphi_m] \rangle$ and the X-ray intensity distribution in reciprocal space were expressed by nine parameters representing the fault probability. Then, from the formula for the intensity distribution, the influence of the stacking faults on the peak integrated intensity, integral breadth, peak shifts and peak asymmetry were found. One of the faults, the intrinsic-$2h$ stacking fault, was investigated by Prager (1977) in AgI crystals. Using this theory, Lele (1974) solved the problem of X-ray diffraction from $6H(33)$, $9R(12)_3$ and $12R(13)_3$ structures with stacking faults. However, only some particular cases of the faults were considered. This theory has not found a wide use for other polytypic structures because of the too complicated calculations.

Very useful simplifications of the theory were possible due to Hollway's (1969) method of analytic solution. This method, based on Wilson's (1942) equation, expressed the diffracted intensity directly in terms of the coefficients of the characteristic equation and the boundary conditions. Applying this method to Prasad & Lele's (1971) theory, Pandey & Krishna (1976) described the X-ray diffraction by $6H(33)$ structure containing all 14 possible types of intrinsic faults. Some modifications of this method and adoption to $8H(44)$ and $nH(\frac{n}{2}\frac{n}{2})$ structures were presented by Michalski, Demianiuk, Kaczmarek & Zhmija (1981*a*, *b*) and some faults in $4H$, $6H(33)$ and $8H(44)$ crystals were investigated (Michalski, Demianiuk, Kaczmarek & Zhmija, 1980, 1982).

In the general theory presented below all single stacking faults in an arbitrary n-periodical close-packed polytypic structures are considered. The single stacking faults in $3C$ (intrinsic and twin or growth faults) and $2H$ (deformation and growth faults) structures are also considered in this theory.

2. The initial equations

In the notation used by Warren (1959), the diffracted intensity from a close-packed crystal with stacking faults can be written as

$$I(h_3)=\psi^2\sum_{m=-\infty}^{+\infty}\langle \exp(i\varphi_m)\rangle \exp[2\pi i(m/n)h_3], \quad (1)$$

where h_3 is the coordinate of the reciprocal space along various dimensions of the unit cell, n is a period of identity of structure in this direction, ψ^2 is a factor independent of the faultiness of the structure, φ_m is the phase difference across a pair of mth-neighbour layers, and $\langle \exp(i\varphi_m)\rangle$ is the average value of the phase factors evaluated from all pairs of mth-neighbour layers.

In (1) the faultiness of the structure is taken into consideration only in the factor $\langle \exp(i\varphi_m)\rangle$. Therefore, finding the intensity distribution in reciprocal space was usually started by expressing this factor in terms of faultiness parameters. However, as follows from the work of Holloway (1969) and Pandey & Krishna (1976), the evaluation of $\langle \exp(i\varphi_m)\rangle$ is not necessary for finding the intensity distribution in reciprocal space. It is sufficient that the average phase factor $\langle \exp(i\varphi_m)\rangle$ may be expressed in the form

$$\langle \exp(i\varphi_m)\rangle=\sum_{j=1}^{n}K_jX_j^m, \quad (2)$$

where the X_j are the roots of the so-called characteristic equation, which, in general, has the form

$$a_nX^n+a_{n-1}X^{n-1}+\ldots+a_0=0, \quad (3)$$

and K_j are the roots of the set of equations

$$J(m)=\sum_{j=1}^{n}K_jX_j^m, \quad m=1,2,\ldots,n, \quad (4)$$

where $J(m)$ are the so-called boundary conditions [values of $\langle \exp(i\varphi_m)\rangle$ for $m=0, 1, 2, \ldots, n$].

Then the intensity distribution in reciprocal space may be expressed in terms of the coefficients a_j of the characteristic equation and boundary conditions $J(m)$, without the solution of (3) and the set of equations (4). From Holloway (1969), (1) can be written as

$$I(h_3)=\psi^2\times\left\{\frac{1}{2}+\frac{\sum_{j=1}^{n-1}\sum_{k=0}^{j-1}a_{n-k}J(j-k)\exp[(n-j)(i2\pi/n)h_3]-a_0}{\sum_{j=0}^{n}a_j\exp[ij(2\pi/n)h_3]}\right\}$$
$$+\text{complex conjugate}. \quad (5)$$

However, complete expressions for the coefficients a_j, boundary conditions $J(m)$ and intensity distribution are also not necessary for describing the changes in the intensity distribution. As will be shown in the next section, the main measurable parameters describing the changes caused by faultiness may be evaluated by using only some terms of a_j and $J(m)$. These terms have been expressed by fault probabilities for arbitrary n-periodical structure assuming small values of these probabilities.

3. Stacking faults in arbitrary *n*-periodical structure

For the simplest close-packed structures $3C$ and $2H$ the stacking of layers in the unit cell is sufficiently characterized by the symbols A, B and C. In polytypic structures the symbols A, B and C can be repeated on the different positions of the same unit cells. Therefore let us denote additionally the successive layers of each of three perfect primary sequences (originating from the A-, B- or C-type layers) by subscript j ($j = 1, 2, \ldots, n$; where n is a period of identity of structure). For twinned sequences (enantiomorphous with the primary one) we use subscript j and a prime. Next we denote the probability of obtaining a faulted layer with subscript k (or k') after a layer with subscript j by α_{jk} (or $\alpha_{jk'}$). Subsequently, the probabilities of obtaining perfect layers with subscripts $(j+1)$ next to layers with subscripts j are given by symbols $(1-g_j)$ or $(1-g_{j'})$, where

$$g_j = \sum_{k=1}^{n} \alpha_{jk} \quad \text{and} \quad g_{j'} = \sum_{k=1}^{n} \alpha_{jk'}. \tag{6}$$

The classification, used in the literature, of stacking faults in close-packed structures divides them into deformation and growth faults (Lele, 1974; Frey & Boysen, 1981). This distinction is based on the process of fault formation. The faults which can arise through the process of glide of one part of the crystal with respect to the rest of it are called deformation faults, and the faults which can arise only from a growth mechanism are called growth faults.

In § 4 of this paper it will be shown that another distinction with regard to the general theory of X-ray diffraction is more convenient. All the possible single stacking faults for arbitrary n-periodical close-packed polytypic structures can be divided into twinning and non-twinning faults.

The method of defining all the possible single stacking faults (twinning and non-twinning) in arbitrary close-packed polytypic structures is illustrated by Figs. 1(a) and (b). For some layers in Figs. 1(a) and (b) we cannot assign the symbols A, B or C by the general method for all polytypic structures. In order to obviate this difficulty in the notation of these layers, we introduce the symbols X_j^A, X_j^B, X_j^C and X_j, where $j = 1, 2, \ldots, n$ (see Fig. 2). The superscripts A, B or C indicate here that the layer is taken from the sequence originating from A-, B- or C-type layers. Absence of superscripts from the symbol X means that we do not know from which sequence the layer with subscript j is taken. For example, layers lying immediately after faults can be denoted only by these symbols.

From Figs. 1 and 2 it follows that non-twinning faults can occur in all polytypic structures, whereas twinning faults can only occur in structures with non-symmetrical distribution of sign, '+' and '−' in

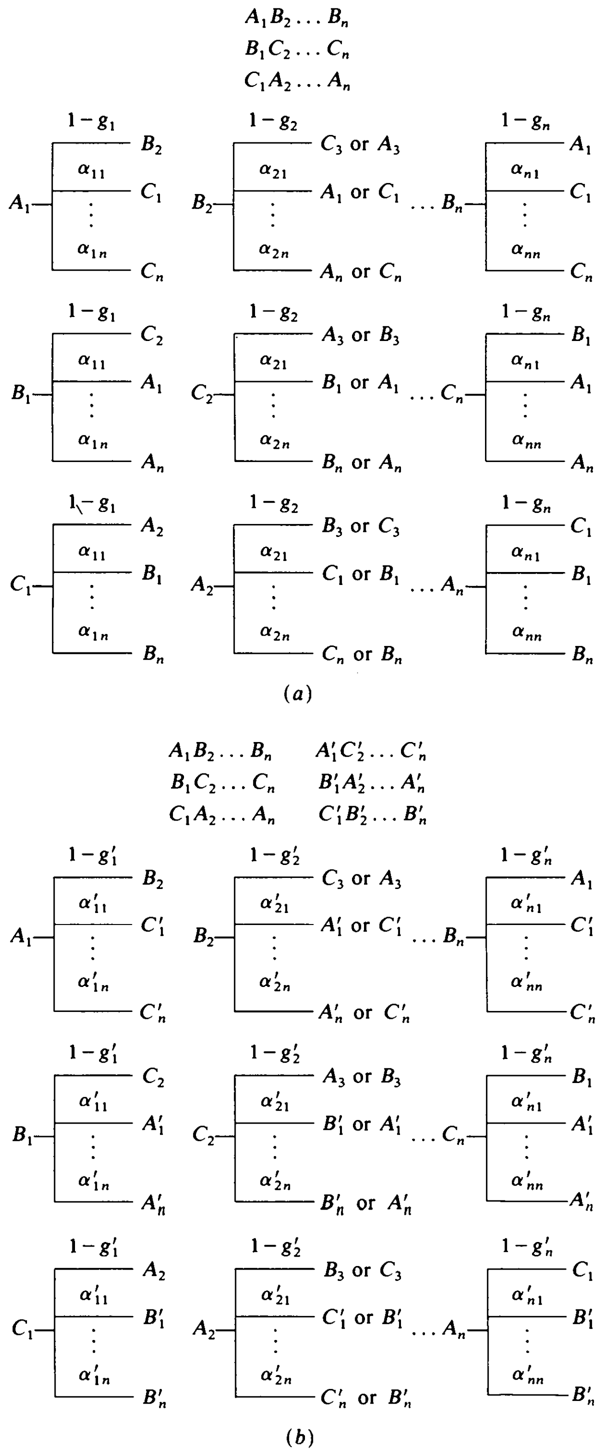

Fig. 1. (a) All the possible single non-twinning faults in arbitrary close-packed structures. (b) All the possible single twinning faults in arbitrary close-packed structures.

Hägg's symbols. Moreover, all the twinning faults are growth faults, while among the non-twinning faults we can distinguish growth and deformation faults.

Besides the single stacking faults considered above, there are double, triple and multiple faults. For instance, single(intrinsic)-, double(extrinsic)-, triple- and multiple-deformation faults in $3C$ crystals were considered by Kakinoki (1967). Moreover, the fault $ABAB:C:ABAB$ in the $2H$ structure was called the extrinsic fault by Pandey & Krishna (1977). The names intrinsic and extrinsic faults were also used (Prasad & Lele, 1971; Lele, 1974; Pandey & Krishna, 1976) for polytypic crystals together with deformation and growth faults. According to our distinction, the name intrinsic relates in these cases to single non-twinning faults, the name extrinsic relates to double non-twinning faults and the name extrinsic in the $2H$ structure relates to double non-twinning–twinning faults.

4. Coefficients of the characteristic equation

In the notation used by Warren (1959) the average phase factor $\langle \exp(i\varphi_m)\rangle$ can be expressed, in general, by

$$\langle \exp(i\varphi_m)\rangle = P_m^0 + P_m^+ \exp[\pm 2\pi i(H-K)/3] + P_m^- \exp[\mp 2\pi i(H-K)/3]. \quad (7)$$

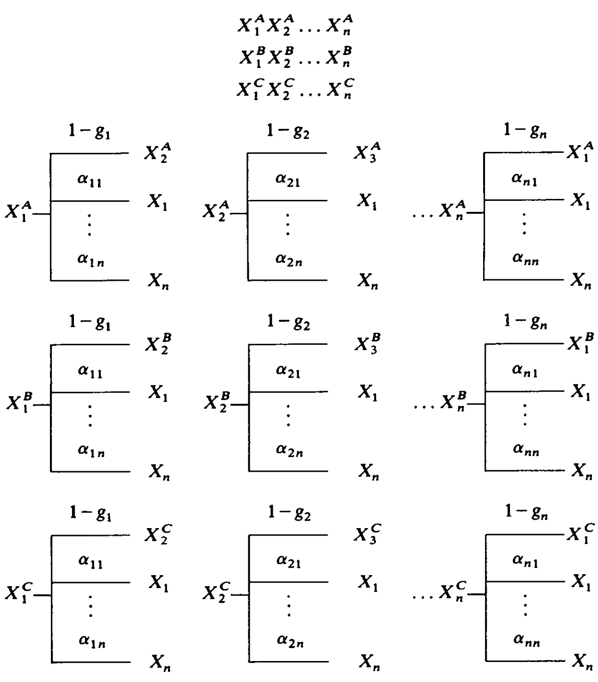

Fig. 2. The X_j^A, X_j^B, X_j^C and X_j symbols introduced for notation of layers in close-packed structures.

For $H-K=1$, (7) has the form

$$\langle \exp(i\varphi_m)\rangle = P_m^0 + P_m^+ \exp(\pm 2\pi i/3) + P_m^- \exp(\mp 2\pi i/3), \quad (8)$$

where P_m^0, P_m^+, P_m^- are the probabilities that, relative to the zero layer, the layer m is the same, or one ahead, or one behind in the ABC sequence.

Let us introduce the subscripts j and k defining the faults into a description of X-ray diffraction. If the origin layer has symbol A, the probabilities P_m^0, P_m^+ and P_m^- can be written as

$$P_m^0 = \sum_{j=1}^n P(m, A_j), \qquad P_m^+ = \sum_{j=1}^n P(m, B_j)$$

and

$$P_m^- = \sum_{j=1}^n P(m, C_j), \quad (9)$$

where $P(m, A_j)$, $P(m, B_j)$ and $P(m, C_j)$ are probabilities of occurrence of the layers A_j, B_j and C_j type on m position. Substituting (9) in (8), we can write

$$\langle \exp(i\varphi_m)\rangle = \sum_{j=1}^n P(m, A_j)\exp[i\varphi(m, A_j)] + \sum_{j=1}^n P(m, B_j)\exp[i\varphi(m, B_j)] + \sum_{j=1}^n P(m, C_j)\exp[i\varphi(m, C_j)], \quad (10)$$

where $\varphi(m, A_j)=0$, $\varphi(m, B_j)=2\pi i/3$ and $\varphi(m, C_j)=-2\pi i/3$ are phases of layers of type A_j, B_j and C_j. The terms with identical subscripts on the right-hand side of (10) may be grouped and written as

$$P(m, A_j)\exp[i\varphi(m, A_j)] + P(m, B_j)\exp[i\varphi(m, B_j)] + P(m, C_j)\exp[i\varphi(m, C_j)] = \langle \exp[i\varphi(m, X_j)]\rangle, \quad j=1,2,\ldots,n, \quad (11)$$

where $\langle \exp[i\varphi(m, X_j)]\rangle$ means the average value of phase factors for layers with subscript j on the m positions. Thus the average phase factor $\langle \exp(i\varphi_m)\rangle$ may be expressed in the form

$$\langle \exp(i\varphi_m)\rangle = \sum_{j=1}^n \langle \exp[i\varphi(m, X_j)]\rangle. \quad (12)$$

Recurrence relations for the average phase factors $\langle \exp[i\varphi(m, X_j)]\rangle$ may be formed using the probability trees presented in Fig. 3. The $3n$ types of layers X_j^A, X_j^B and X_j^C (where $j=1, 2, \ldots, n$) can occur on an arbitrary position in the crystal. Let the probabilities of occurrence of these layers on position $(m-1)$ be respectively equal to $P(m-1, X_j^A)$, $P(m-1, X_j^B)$ and $P(m-1, X_j^C)$. Hence the probabilities $P(m, X_j)$ can be expressed as

$$\begin{aligned}P(m, X_k) = &(1-g_{k-1})P(m-1, X^A_{k-1})\\ &+\sum_{j=1}^{n} \alpha_{jk} P(m-1, X^A_j)\\ &+(1-g_{k-1})P(m-1, X^B_{k-1})\\ &+\sum_{j=1}^{n} \alpha_{jk} P(m-1, X^B_j)\\ &+(1-g_{k-1})P(m-1, X^C_{k-1})\\ &+\sum_{j=1}^{n} \alpha_{jk} P(m-1, X^C_j),\\ &\qquad k=1,2,\ldots,n. \qquad (13)\end{aligned}$$

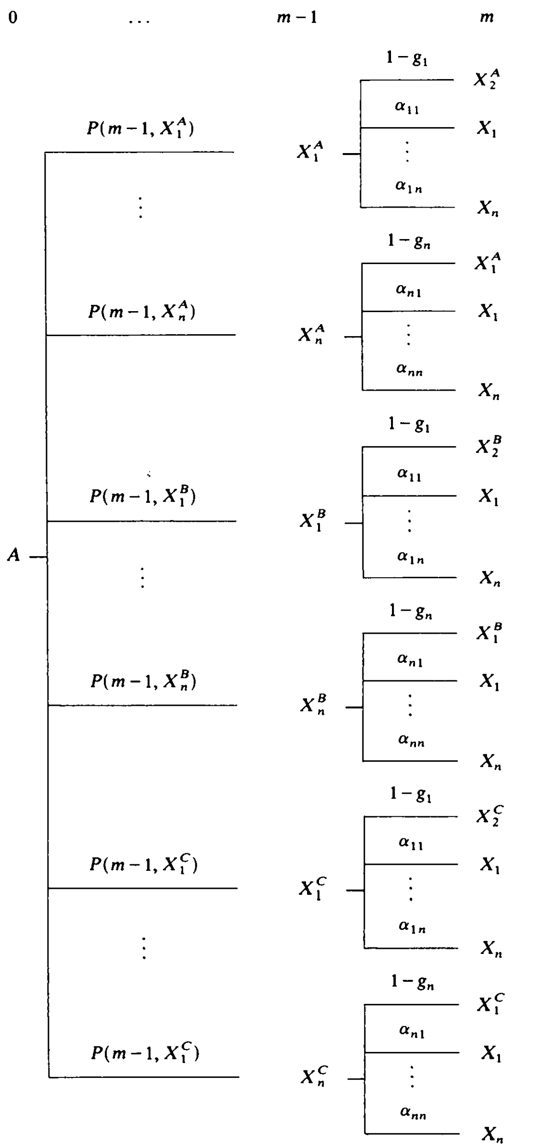

Fig. 3. Probability trees for all the possible layers on $(m-1)$ and m positions in the sequences originating from A-type layers of close-packed structures.

The average phase factor $\langle\exp[i\varphi(m, X_k)]\rangle$ can be obtained by multiplying each of the $(3n+3)$ terms on the right-hand side of (13) by the phase factor of the layer on position m described by this term. In order to evaluate enough phases let us consider them as sums of the phases of layers on positions $(m-1)$ and changes of phase from position $(m-1)$ to m. Phases of layers on position $(m-1)$ are found because the subscripts j and superscripts A, B or C are known for these layers. The changes of phase can be determined by using Hägg's structure symbols. For this purpose let us introduce the so-called phase-change factor after layers with subscript j,

$$S_j = \exp(\pm 2\pi i/3), \qquad (14)$$

where the sign '+' or '−' is chosen by Hägg's structure symbols. The change of phase is in agreement with Hägg's structure symbol if a perfect layer occurs after a layer with subscript j. The change of phase is opposite to Hägg's structure symbol if a faulted layer occurs after a layer with subscript j. In general the factor S_j has the properties

$$S_j^2 = S_j^*, \quad S_{j+n} = S_j \quad \text{and} \quad \prod_{j=1}^{n} S_j = 1, \qquad (15)$$

where S_j^* is the complex conjugate of S_j.

After multiplication on the right-hand side of (13) we can write

$$\begin{aligned}&\langle\exp[i\varphi(m, X_k)]\rangle\\ &\quad=(1-g_{k-1})S_{k-1}P(m-1, X^A_{k-1})\\ &\qquad\times\exp[i\varphi(m-1, X^A_{k-1})]\\ &\qquad+\sum_{j=1}^{n}\alpha_{jk}S_j^* P(m-1, X^A_j)\exp[i\varphi(m-1, X^A_j)]\\ &\qquad+(1-g_{k-1})S_{k-1}P(m-1, X^B_{k-1})\\ &\qquad\times\exp[i\varphi(m-1, X^B_{k-1})]\\ &\qquad+\sum_{j=1}^{n}\alpha_{jk}S_j^* P(m-1, X^B_j)\exp[i\varphi(m-1, X^B_j)]\\ &\qquad+(1-g_{k-1})S_{k-1}P(m-1, X^C_{k-1})\\ &\qquad\times\exp[i\varphi(m-1, X^C_{k-1})]\\ &\qquad+\sum_{j=1}^{n}\alpha_{jk}S_j^* P(m-1, X^C_j)\\ &\qquad\times\exp[i\varphi(m-1, X^C_j)], \qquad k=1,2,\ldots,n. \qquad (16)\end{aligned}$$

The terms with the same subscripts on the right-hand side of (16) may be grouped and written as

$$\begin{aligned}&P(m-1, X^A_j)\exp[i\varphi(m-1, X^A_j)]\\ &\quad+P(m-1, X^B_j)\exp[i\varphi(m-1, X^B_j)]\\ &\quad+P(m-1, X^C_j)\exp[i\varphi(m-1, X^C_j)]\\ &\qquad=\langle\exp[i\varphi(m-1, X_j)]\rangle, \quad j=1,2,\ldots,n. \qquad (17)\end{aligned}$$

Thus we obtain the following set of recurrence relations:

$$\begin{aligned}\langle \exp[i\varphi(m, X_k)]\rangle &= (1-g_{k-1})S_{k-1}\langle \exp[i\varphi(m-1, X_{k-1})]\rangle \\ &\quad + \sum_{j=1}^{n} \alpha_{jk}S_j^*\langle \exp[i\varphi(m-1, X_j)]\rangle,\end{aligned}$$

$$k = 1, 2, \dots, n. \quad (18)$$

Let the solution of the relations (18) have the form

$$\langle \exp[i\varphi(m, X_j)]\rangle = K_j X^m, \quad j = 1, 2, \dots, n. \quad (19)$$

Substituting (19) into (18) we obtain the set of n equations for coefficients K_j:

$$K_k X - (1-g_{k-1})S_{k-1}K_{k-1} - \sum_{j=1}^{n} \alpha_{jk}S_j^* K_j = 0,$$

$$k = 1, 2, \dots, n. \quad (20)$$

The set of equations (20) can be written in matrix form as

$$\begin{bmatrix} \alpha_{11}S_1^* - X & \alpha_{21}S_2^* & \alpha_{31}S_3^* & \cdots & \alpha_{n1}S_n^* + (1-g_n)S_n \\ \alpha_{12}S_1^* + (1-g_1)S_1 & \alpha_{22}S_2^* - X & \alpha_{32}S_3^* & \cdots & \alpha_{n2}S_n^* \\ \alpha_{13}S_1^* & \alpha_{23}S_2^* + (1-g_2)S_2 & \alpha_{33}S_3^* - X & \cdots & \alpha_{n3}S_n^* \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ \alpha_{1n}S_1^* & \alpha_{2n}S_2^* & \alpha_{3n}S_3^* & \cdots & \alpha_{nn}S_n^* - X \end{bmatrix} \begin{bmatrix} K_1 \\ K_2 \\ K_3 \\ \vdots \\ K_n \end{bmatrix} = 0. \quad (21)$$

For non-trivial values of K_j solutions, the determinant of the first matrix of (21) must vanish. From this condition the characteristic equation is obtained. Expanding the determinant under the assumption of small values of α_{jk} we can neglect all terms which contain products of different α_{jk} or powers of α_{jk} greater than one. Thus the determinant of the $n \times n$ matrix with all non-zero terms can be substituted by the sum of n determinants which contain only one type of α_{jk} at a time, whereas the other terms with α_{mn} $(m \neq j, n \neq k)$ are equal to zero.

For particular $\alpha_{jk} \neq 0$ we have the following cases: when $k \leq j$,

$$X^n - S_j^* \prod_{i=k}^{j-1} S_i \alpha_{jk} X^{n+k-j-1} + \alpha_{jk} - 1 = 0; \quad (22)$$

when $k > j$,

$$X^n - S_j^* \prod_{i=j}^{k-1} S_i^* \alpha_{jk} X^{k-j-1} + \alpha_{jk} - 1 = 0. \quad (23)$$

In the recurrence relations for the twinning faults it is also necessary to consider the fact that these faults change the sequence of layers after the fault into having a twin relationship with the primary one. For the primary sequence the phase factors of layers with particular subscripts k are given by

$$\begin{aligned}\exp[i\varphi(X_k^A) - i\varphi(A)] &= \exp[i\varphi(X_k^B) - i\varphi(B)] \\ &= \exp[i\varphi(X_k^C) - i\varphi(C)] \\ &= \prod_{i=1}^{k-1} S_i, \end{aligned} \quad (24)$$

while for the twinned sequence

$$\begin{aligned}\exp[i\varphi(X_{k'}^A) - i\varphi(A)] &= \exp[i\varphi(X_{k'}^B) - i\varphi(B)] \\ &= \exp[i\varphi(X_{k'}^C) - i\varphi(C)] \\ &= \prod_{i=1}^{k-1} S_i^*. \end{aligned} \quad (25)$$

Combining (25) and (24) we can write

$$\begin{aligned}\exp[i\varphi(X_{k'}^A) - i\varphi(X_k^A)] &= \exp[i\varphi(X_{k'}^B) - i\varphi(X_k^B)] \\ &= \exp[i\varphi(X_{k'}^C) - i\varphi(X_k^C)] \\ &= \prod_{i=1}^{k-1} S_i^*/S_i = \prod_{i=1}^{k-1} S_i. \end{aligned} \quad (26)$$

In order to obtain the recurrence relations for the twinning faults it is necessary to multiply all terms [of (18)] containing probabilties α_{jk} by the factors expressed by (26).

For $\alpha_{jk} \neq 0$ the characteristic equations obtained as for (22) and (23) have the following forms: when $k \leq j$,

$$X^n - S_j^* \prod_{i=1}^{j-1} S_i \alpha_{jk'} X^{n+k-j-1} + \alpha_{jk'} - 1 = 0; \quad (27)$$

when $k > j$,

$$X^n - S_j^* \prod_{i=1}^{j-1} S_i \alpha_{jk'} X^{k-j-1} + \alpha_{jk'} - 1 = 0. \quad (28)$$

In general, (22), (23), (27) and (28) have complex coefficients. However, they are separable into equations with real and imaginary coefficients, and the latter equations may be omitted.

5. Boundary conditions

By analogy with Prasad & Lele (1971), we derive expressions for the boundary conditions from the equation

$$\langle \exp[i\varphi_m]\rangle = J(m) = \sum_{j=1}^{n} w_j J(m)_j,$$

$$m = 0, 1, 2, \dots, n, \quad (29)$$

where w_j represents the probability of occurrence of layers with a particular value of j at an arbitrary position in the crystal and $J(m)_j$ are the average phase factors for layers on position m in sequences originating from a layer with a particular subscript j.

For small values of α_{jk}, the boundary conditions $J(m)$ can be written as the sums of terms $J^0(m)$

without α_{jk} and the terms $J'(m)$ containing α_{jk}, as

$$J(m)=J^0(m)+J'(m). \tag{30}$$

It will be shown in § 6 that only the terms $J^0(m)$ are needed for obtaining the final expressions. The terms $J^0(m)$ are determined as

$$J^0(m)=\sum_{j=1}^{n} w_j^0 J^0(m)_j. \tag{31}$$

where the superscript '0' denotes the term without α_{jk}.

To obtain w_j^0 the following set of equations can be obtained from Fig. 3:

$$w_k^0=(1-g_{k-1})w_{k-1}^0, \quad k=1,2,\ldots,n, \tag{32}$$

with the normalizing condition

$$\sum_{j=1}^{n} w_j^0=1. \tag{33}$$

The solution of (32) and (33) is

$$w_1^0=w_2^0=\ldots=w_n^0=1/n. \tag{34}$$

In order to evaluate $J^0(m)_j$ it is sufficient to consider the perfect sequences because only for them are the probabilities of occurrence of the layer on position m equal to unity without any α_{jk}. Thus the terms $J^0(m)_j$ are equal to the phase factors of layers on positions m in perfect sequences and can be written as

$$J^0(m)_j=\prod_{i=j}^{j+m-1} S_i \quad \text{for} \quad m>0 \quad \text{and} \quad J^0(0)_j=1. \tag{35}$$

From (31), (34) and (35), the terms of boundary conditions without α_{jk} can be written as

$$J^0(m)=\frac{1}{n}\sum_{j=1}^{n}\prod_{i=j}^{j+m-1} S_i \quad \text{for} \quad m>0 \quad \text{and} \quad J^0(0)=1. \tag{36}$$

Moreover, it can be shown that the terms of the boundary conditions without α_{jk} have the following symmetry:

$$J^0(m)=J^0(n-m)^*=J^0(n+m). \tag{37}$$

Owing to the above symmetry further considerations will be simplified.

6. Influence of stacking faults on the reciprocal-lattice point shifts, broadenings and changes in the peak maxima

Taking into account the fact that in general the boundary conditions $J(m)$ are complex and the coefficients a_j of the characteristic equation are real, we can rearrange (5) for the intensity distribution into the simple form

$$I(h_3)=\psi^2 \times\left(1+\frac{2\sum_{m=0}^{n}\{\operatorname{Re} N_m\cos[(2m\pi/n)h_3]+\operatorname{Im} N_m\sin[(2m\pi/n)h_3]\}}{\sum_{m=0}^{n} D_m\cos[(2m\pi/n)h_3]}\right) \tag{38}$$

where Re N_m and Im N_m mean the real and the imaginary parts of N_m and

$$\begin{aligned}
D_0&=(1+a_{n-1}^2+\ldots+a_0^2),\\
D_1&=2(a_{n-1}+a_{n-1}a_{n-2}+\ldots+a_1a_0), \quad \ldots \quad ,\\
D_{n-2}&=2(a_2+a_{n-1}a_1+a_{n-2}a_0),\\
D_{n-1}&=2(a_1+a_{n-1}a_0), \qquad D_n=2a_0,\\
N_0&=a_{n-1}J(1)+a_{n-2}[J(2)+a_{n-1}J(1)]\\
&\quad+a_{n-3}[J(3)+a_{n-1}J(2)+a_{n-2}J(1)]+\ldots\\
&\quad+a_1[J(n-1)+a_{n-1}J(n-2)+\ldots+a_2J(1)]\\
&\quad-a_0^2,\\
N_1&=a_{n-2}J(1)+a_{n-3}[J(2)+a_{n-1}J(1)]+\ldots\\
&\quad+a_0[J(n-1)+a_{n-1}J(n-2)+\ldots+a_2J(1)]\\
&\quad+a_nJ(1)+a_{n-1}[J(2)+a_{n-1}J(1)]+\ldots\\
&\quad+a_2[J(n-1)+a_{n-1}J(n-2)+\ldots+a_2J(1)]\\
&\quad-a_1a_0, \quad \ldots \quad ,\\
N_{n-2}&=a_1J(1)+a_0[J(2)+a_{n-1}J(1)]\\
&\quad+a_n[J(n-2)-a_{n-1}J(n-3)+\ldots+a_3J(1)]\\
&\quad+a_{n-1}[J(n-1)+a_{n-1}J(n-2)+\ldots\\
&\quad+a_2J(1)]-a_{n-2}a_0,\\
N_{n-1}&=a_0J(1)+a_n[J(n-1)+a_{n-1}J(n-2)+\ldots\\
&\quad+a_2J(1)]-a_{n-1}a_0,\\
N_n&=-a_0.
\end{aligned} \tag{39}$$

If the boundary conditions are real (this is true, for example, for hexagonal structures) (38) has the form

$$I(h_3)=\psi^2\left\{1+\frac{2\sum_{m=0}^{n} N_m\cos[(2m\pi/n)h_3]}{\sum_{m=0}^{n} D_m\cos[(2m\pi/n)h_3]}\right\}. \tag{40}$$

To describe the shifts $\Delta h_3(h_3)$ of the reciprocal-lattice points caused by stacking faults, let us substitute $(h_3+\Delta h_3)$ into (38) as argument. Differentiating this expression with respect to Δh_3 and equating to zero, we obtain for Δh_3 the equation

$$\sum_{m=0}^{n} \{m \operatorname{Re} N_m \sin[(2m\pi/n)h_3+(2m\pi/n)\Delta h_3] - m \operatorname{Im} N_m \cos[(2m\pi/n)h_3+(2m\pi/n)\Delta h_3]\} \times \sum_{m=0}^{n} D_m \cos[(2m\pi/n)h_3+(2m\pi/n)\Delta h_3] - \sum_{m=0}^{n} mD_m \sin[(2m\pi/n)h_3+(2m\pi/n)\Delta h_3] \times \sum_{m=0}^{n} \{\operatorname{Re} N_m \cos[(2m\pi/n)h_3+(2m\pi/n)\Delta h_3] + \operatorname{Im} N_m \sin[(2m\pi/n)h_3+(2m\pi/n)\Delta h_3]\} = 0. \quad (41)$$

If we expand the sine and cosine functions into series, use (22), (23), (27), (28) and (39) and assume small values of α_{jk}, the solution Δh_3 can be expressed as

$$\Delta h_3(h_3) = (1/4n\pi) \sum_{m=0}^{n} mD_m \sin[(2m\pi/n)h_3]. \quad (42)$$

After substitution of (32), (33) and (39) into (42), the expression for $\Delta h_3(h_3)$ has the final form

$$\Delta h_3(h_3, \alpha_{jk}) = (1/2\pi)\alpha_{jk} \operatorname{Re} S_{jk} \times \sin\{[2(k-j-1)\pi/n]h_3\}, \quad (43)$$

where

$$S_{jk} = \begin{cases} \left.\begin{array}{ll} S_j^* \prod_{i=k}^{j-1} S_i & \text{for } k \le j \\ S_j^* \prod_{i=j}^{k-1} S_i^* & \text{for } k > j \end{array}\right\} \text{in the case of non-twinning faults,} \\ S_j^* \prod_{i=1}^{j-1} S_i \quad \text{in the case of twinning faults.} \end{cases} \quad (44)$$

The broadenings $\Delta w(h_3)$ of the reciprocal-lattice points caused by stacking faults are calculated as their half widths, determined by

$$I(h_3+\Delta h_3+\Delta w/2) = \tfrac{1}{2} I(h_3+\Delta h_3). \quad (45)$$

Putting $(h_3+\Delta h_3+\Delta w/2)$ and $(h_3+\Delta h_3)$ as argument into (38) and expanding cosine and sine functions into series, we obtain from (45) the equation for Δw. According to considerations given in the Appendix, for small α_{jk} the numerators of fractions on both sides of this equation are equal to each other and for the evaluation of $\Delta w(h_3)$ it is sufficient to compare the denominators.

Consequently we obtain for Δw the equation

$$\sum_{m=0}^{n} D_m\{\cos[(2m\pi/n)h_3] - (2m\pi/n)(\Delta h_3+\Delta w/2) \sin[(2m\pi/n)h_3] - \tfrac{1}{2}(2m\pi/n)^2(\Delta h_3+\Delta w/2)^2 \cos[(2m\pi/n)h_3]\} = 2 \sum_{m=0}^{n} D_m\{\cos[(2m\pi/n)h_3] - (2m\pi/n)\Delta h_3 \sin[(2m\pi/n)h_3] - \tfrac{1}{2}[(2m\pi/n)\Delta h_3]^2 \cos[(2m\pi/n)h_3]\}. \quad (46)$$

The solution of (46) has the form

$$\Delta w(h_3) = (1/\pi)\left\{\sum_{m=0}^{n} D_m \cos[(2m\pi/n)h_3] - 4\pi^2(\Delta h_3)^2\right\}^{1/2}. \quad (47)$$

Substituting (32), (33) and (39) in (47) we obtain finally

$$\Delta w(h_3, \alpha_{jk}) = (\alpha_{jk}/\pi)[1+(\operatorname{Re} S_{jk})^2 - 2 \operatorname{Re} S_{jk} \cos\{[2(k-j-1)\pi/n]h_3\} - (\operatorname{Re} S_{jk})^2 \sin^2\{[2(k-j-1)\pi/n]h_3\}]^{1/2}, \quad (48)$$

where S_{jk} is determined by (44).

The influence of a particular α_{jk} on $I_{\max}(h_3)$ may be found from the formula

$$I_{\max}(h_3) = I(h_3+\Delta h_3). \quad (49)$$

From the Appendix, the final formula for $I_{\max}(h_3, \alpha_{jk})$ has the following form:

(i) in the case of structures for which the terms $J^0(m)$ of boundary conditions are real,

$$I_{\max}(h_3, \alpha_{jk}) = \psi^2 \frac{L'(h_3, \alpha_{jk})}{\pi^2[\Delta w(h_3, \alpha_{jk})]^2}, \quad (50)$$

where

$$L'(h_3, \alpha_{jk}) = 2\alpha_{jk}\Big(1 - \operatorname{Re} S_{jk} J^0(j-k+1) + \sum_{m=1}^{n/2-1} \{J^0(m)+J^0(n-m) - \operatorname{Re} S_{jk}[J^0(m-n-k+j+1) + J^0(j+1-k-m)]\} \cos[(2m\pi/n)h_3] + [J^0(n/2) - \operatorname{Re} S_{jk} J^0(j+1-k-n/2)] \cos(\pi h_3)\Big), \quad (51)$$

and $\Delta w(h_3, \alpha_{jk})$ are determined by (48);

(ii) in the case of structures for which the terms $J^0(m)$ are complex,

$$I_{\max}(h_3, \alpha_{jk}) = \psi^2 \frac{L^0(h_3)}{\pi^2[\Delta w(h_3, \alpha_{jk})]^2}, \quad (52)$$

where

$$L^0 = (4/n)\ \mathrm{Im} \sum_{m=0}^{n} \sum_{j=1}^{n} \prod_{i=j}^{j+m-1} S_i \sin[(2m\pi/n)h_3]. \tag{53}$$

7. Discussion

The final formulae (43), (48), (50) and (52) allow us to express the measurable parameters (Δh_3, Δw and $I_{\max}$) of changes in the intensity distribution by fault probabilities for arbitrary n-periodical structure. These formulae are given in the form of simple algebraic and trigonometric functions of the subscripts j, k defining the type of faults, factors S_j determined by the Hägg structure symbols, coordinates h_3 and probabilities α_{jk}.

The subscripts j,k defining the faults are convenient for mathematical treatment of arbitrary n-periodical structures. However, it is possible that faults with identical structures can be denoted by different subscripts j, k. In that case the faults should be considered to repeat the same type of fault and the common diffraction effects should be evaluated. For this reason, for polytypes in which the faults are repeated it is not possible to use the final expressions directly.

The application of the theory to the cases of hexagonal and rhombohedral structures will be presented by Michalski, Kaczmarek & Demianiuk (1988). The physical meaning of the assumption of α_{jk}, for instance of the structures with faults, will also be discussed in that paper.

In the theory presented above only single faults are considered. This case seems to be the most important. As a next step of development of the theory, faults which are not single could be considered. These faults may be defined similarly by groups of indexes. Three indexes would be necessary and sufficient for double faults, four indexes for triple faults, *etc.*

APPENDIX

Derivation of the formulae for $I_{\max}(h_3)$

Substituting the Δh_3 [given by (55)] into (59) and expanding the sine and cosine functions into a series we obtain

$$I_{\max}(h_3) = \psi^2(1 + L/M), \tag{A1}$$

where

$$\begin{aligned} L = 2 \sum_{m=0}^{n} (&\mathrm{Re}\, N_m\{\cos[(2m\pi/n)h_3] \\ &- (2m\pi/n)\Delta h_3 \sin[(2m\pi/n)h_3] \\ &- \tfrac{1}{2}[(2m\pi/n)\Delta h_3]^2 \cos[(2m\pi/n)h_3] + \ldots\} \\ &+ \mathrm{Im}\, N_m\{\sin[(2m\pi/n)h_3] \\ &+ (2m\pi/n)\Delta h_3 \cos[(2m\pi/n)h_3] \\ &- \tfrac{1}{2}[(2m\pi/n)\Delta h_3]^2 \sin[(2m\pi/n)h_3] + \ldots\}), \end{aligned} \tag{A2}$$

$$\begin{aligned} M = \sum_{m=0}^{n} D_m\{&\cos[(2m\pi/n)h_3] \\ &- (2m\pi/n)\Delta h_3 \sin[(2m\pi/n)h_3] \\ &- \tfrac{1}{2}[(2m\pi/n)\Delta h_3]^2 \cos[(2m\pi/n)h_3] + \ldots\}. \end{aligned} \tag{A3}$$

In the denominator the terms without α_{jk} and containing the first power of α_{jk} vanish due to specific symmetry of D_m. After omitting the terms with power of α_{jk} greater than two, we obtain

$$M = \sum_{m=0}^{n} D_m \cos[(2m\pi/n)h_3] - 4\pi^2(\Delta h_3). \tag{A4}$$

In the above formula, particular D_m terms occur effectively in the form of sums $(D_m + D_{n-m})$ because $\cos(2m\pi h_3/n) = \cos[2(n-m)\pi h_3/n]$. Hence we need not evaluate the a_j terms containing α_{jk}^2 in particular D_m terms, because these terms cancel each other.

In the numerator of expression (A1) it is sufficient to take into consideration only the terms with the lowest power of α_{jk}. The terms without α_{jk} occurring in particular N_m can be written as

$$\begin{gathered} N_0^0 = -1, \\ N_1^0 = -J^0(n-1) + J^0(1), \\ N_2^0 = -J^0(n-2) + J^0(2), \\ N_{n/2}^0 = 0, \quad \ldots \quad, N_{n-2}^0 = -J^0(2) + J^0(n-2), \\ N_{n-1}^0 = -J^0(1) + J^0(n-1), \quad N_n^0 = 1. \end{gathered} \tag{A5}$$

Separating the real from imaginary parts, we obtain

$$\begin{gathered} \mathrm{Re}\, N_0^0 = -1, \\ \mathrm{Re}\, N_1^0 = \mathrm{Re}\, N_2^0 = \ldots = \mathrm{Re}\, N_{n-1}^0 = 0, \\ \mathrm{Re}\, N_n^0 = 1 \end{gathered} \tag{A6}$$

and

$$\begin{gathered} \mathrm{Im}\, N_0^0 = 0, \quad \mathrm{Im}\, N_1^0 = 2\,\mathrm{Im}\, J^0(1), \\ \mathrm{Im}\, N_2^0 = 2\,\mathrm{Im}\, J^0(2), \quad \ldots \quad, \\ \mathrm{Im}\, N_{n-1}^0 = 2\,\mathrm{Im}\, J^0(n-1), \quad \mathrm{Im}\, N_n^0 = 0. \end{gathered} \tag{A7}$$

Using (A6) and (A7) we can express the terms with the lowest power of α_{jk} of the numerator of (A1) as follows:

(i) in the case of structures with complex boundary conditions,

$$L^0(h_3)=2\sum_{m=0}^{n}\operatorname{Im} N_m^0 \sin[(2m\pi/n)h_3]$$
$$=4\sum_{m=0}^{n}\operatorname{Im} J^0(m)\sin[(2m\pi/n)h_3]; \quad (A8)$$

(ii) in the case of structures with real boundary conditions,

$$L'=2\sum_{m=0}^{n} N'_m\cos[(2m\pi/n)h_3], \qquad (A9)$$

where the prime indicates that the terms contain the first power of α_{jk}. Moreover, in ($A1$) we can omit the unity before the fraction because this one has the same magnitude as α^{-1} in the first case and as α^{-2} in the second case.

In order to evaluate L', we use the fact that N'_m effectively occurs in ($A9$) as $(N'_m+N'_{n-m})$. Thus from (39) it follows that the evaluation of $J'(m)$ is dispensable because they cancel out.

Substituting (39) into ($A9$) we obtain

$$\begin{aligned}L'(h_3)&=2\left\{N'_0+N'_m+\sum_{m=1}^{n/2-1}(N'_m+N'_{n-m})\right.\\&\quad\left.\times\cos[(2m\pi/n)h_3]+N'_{n/2}\cos(\pi h_3)\right\}\\&=2\left(a'_0+a'_jJ^0(n-j)\right.\\&\quad+\sum_{m=1}^{n/2-1}\{a'_0[J^0(m)+J^0(n-m)]\\&\quad+a'_j[J^0(m-j)+J^0(n-m-j)]\}\\&\quad\times\cos[(2m\pi/n)h_3]\\&\quad\left.+[a'_0J^0(n/2)+a'_jJ^0(n/2-j)]\cos(\pi h_3)\right).\end{aligned} \qquad (A10)$$

Using (22), (23), (27) and (28), we can obtain the final formula, (51).

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