X-ray Diffraction from Close-Packed Structures with Stacking Faults

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(Received October 15, 1981)

Abstract

For two types of difference equations for close-packed structures with stacking faults, one was introduced by Wilson [Proc. Roy. Soc. (1942), A**180**, 277] and the other was done by Prasad and Lele [Acta Cryst. (1971), A**27**, 54], the former one is shown to be derived by **P** matrix of Kakinoki & Komura [Acta Cryst. (1964), **19**, 137] and the latter one is done similarly by **Q** matrix of Allegra [Acta Cryst. (1964), **17**, 579]. By solving the characteristic equation of **Q** matrix, the intensity distribution, the integrated intensity, the intensity maximum position, the integrated breadth and the center of gravity for a peak in a diffraction pattern of close-packed structure with stacking faults are formulated.

1. Introduction

Calculation of X-ray diffraction intensity from a close-packed structure with stacking faults is carried out either by the use of difference equation originated by Wilson (1942) or by means of matrix intensity equation introduced by Hendricks & Teller (1942). Difference equations so far appeared in literatures are divided into two kinds, one was introduced by Wilson (1942) and is constructed for the probability of finding a kind of layers, and the other was used by Prasad & Lele (1971) and is constructed by taking into account of phase shifts of layers in addition to the probability. Matrix intensity equation of Hendricks & Teller was improved slightly by Kakinoki & Komura (1949). Then, Allegra (1964) showed that the matrices can be reduced by taking into account of phase shifts between adjacent layers. Allegra's intensity equation is the most easy to deal with close-packed structures with stacking faults. His equation can be obtained directly by changing complexions of layers of Kakinoki & Komura to those of vector sequence as shown by the present author (1976).

The greatest progress in intensity calculation is the study of Gevers (1954), who showed that the intensity could be calculated by the use of the coefficients of characteristic equation of difference equation without solving the characterisic equation. With his method, we can calculate diffraction intensity for higher order

difference equation of which characteristic equation can not be solved algebraically. Applying Gevers's method to matrix intensity equation, Kakinoki & Komura (1965) gave X-ray diffraction intensity equations by which we can calculate the intensity directly if we give the elements of the matrices.

Although we can assure the agreement of the calculated intensities by the both difference equation and matrix intensity methods, the direct derivation of the difference equation from the matrices has not been discussed. In this paper, the present author shows that difference equations of ordinary type can be derived by **P** matrix of Kakinoki & Komura and those of Prasad & Lele (1971) by **Q** matrix of Allegra. At present time, we can solve numerically higher order algebraic equations by electronic computer. By solving numerically the characteristic equation of **Q** matrix, the intensity distribution, the integrated intensity, the intensity maximum position, the integrated breadth and the center of gravity for a peak are formulated in the form of easy calculation by electronic computer. Recently, Lele (1980) gave analytic solution for integrated intensity. His result is examined in this paper for our practical point of view.

2. Ordinary differences equations

Let f_i and P_{ij} be the probabilities defined by Kakinoki & Komura (1965), that is, f_i is the probability finding a layer of ith kind at any position and P_{ij} is the one finding a layer of jth kind after a layer of ith kind. Then, the probability finding a layer of ith kind at the first layer of layer sequence is f_i and the one finding a layer of jth kind at the second layer becomes $\sum_i f_i P_{ij}$. When we form two matrices **F** and **P** as follows, ij element of **F** is f_j and ij element of **P** is P_{ij}, the probability finding a layer of jth kind at the first layer, P_1^j, is $f_j = F_{ij}$, and the one finding the layer of jth kind at the second layer, P^j, becomes

$$\begin{aligned} P_2^j &= \sum_i f_i P_{ij} \\ &= (\mathbf{FP})_{kj} \text{ for any } k \\ &= \sum_i P_1^i P_{ij}. \end{aligned} \tag{1}$$

We have

$$\begin{aligned} P_m^j &= \sum_i (\mathbf{FP}^{m-2})_{ki} P_{ij} \\ &= \sum_i P_m^i P_{ij} \end{aligned} \tag{2}$$

by mathematical induction and taking into account that $(\mathbf{FP}^m)_{ij} = (\mathbf{FP}^m)_{kj}$ for any i and k. From equation (2), we can obtain simultaneous difference equations for P_m^j.

When ith row of **P** is equal to jth row of **P**, $j > i$, we can transform **P** so that the jth row of $\mathbf{APA}^{-1}$ becomes zero. Matrix **A** is given by

$$\mathbf{A} = \mathbf{E} + \mathbf{B}, \tag{3}$$

where **E** is the unit matrix of the same dimension as that of **P** and **B** has -1 as the ji element and zero as the other elements. Since the jth row of **F** becomes zero by the same transformation, the jth row of $\mathbf{FP}^{m-2}$ also becomes zero by the transformation. Hence, we can reduce the number of equations by the transformation.

Example 1.

Howard and Kuwano (1979) gave the **P** matrix of extrinsic faults of second problem of f.c.c. extended by Takahashi (1978) by

$$P_{14} = P_{47} = P_{51} = 1-p, \tag{4a}$$

$$P_{18} = P_{42} = P_{75} = p, \tag{4b}$$

$$P_{27} = P_{34} = P_{51} = P_{67} = P_{84} = P_{91} = 1-q, \tag{4c}$$

$$P_{26} = P_{38} = P_{59} = P_{62} = P_{83} = P_{95} = q. \tag{4d}$$

If we put $p = q$ in equations (4), we obtain **P** matrix of Howard (1977).

To examplify the reduction of the number of equations, we put $p = q$, and rearrange **P** so that the 1st, 2nd and 3rd rows become equal to the 7th, 8th and 9th rows, respectively. Then, we obtain the simultaneous difference equations after the transformation that the 7th, 8th and 9th rows become zero,

$$P_m^1 = P_{m-1}^3(1-p)+P_{m-1}^5(1-p)+P_{m-1}^6 p, \tag{5a}$$

$$P_m^2 = P_{m-1}^1(1-p)+P_{m-1}^4 p+P_{m-1}^6(1-p), \tag{5b}$$

$$P_m^3 = P_{m-1}^2(1-p)+P_{m-1}^4(1-p)+P_{m-1}^5 p, \tag{5c}$$

$$P_m^4 = P_{m-1}^2 p, \tag{5d}$$

$$P_m^5 = P_{m-1}^3 p, \tag{5e}$$

$$P_m^6 = P_{m-1}^1 p. \tag{5f}$$

Substituting equations (5e), (5d) and (5f) into (5a), (5b) and (5c), and rewriting superfices 1, 2 and 3 by A, B and C, respectively, we obtain the three simultaneous equations for P_m^A, P_m^B and P_m^C,

$$P_m^A = P_{m-1}^C(1-p)+P_{m-2}^C+P_{m-2}^A p^2, \tag{6a}$$

$$P_m^B = P_{m-1}^A(1-p)+P_{m-2}^B p^2+P_{m-2}^A(1-p)p, \tag{6b}$$

$$P_m^C = P_{m-1}^B(1-p)+P_{m-2}^B(1-p)p+P_{m-2}^C p^2. \tag{6c}$$

The above simultaneous equations can be solved by putting

$$P_m^i = C_i \rho^m. \tag{7}$$

The characteristic equation is

$$(\rho-1)(\rho+p)^2\{\rho^3+(1-2p)\rho^2+(1-2p)\rho+p(1-3p+3p^2)\} = 0 \tag{8}$$

Although equation (8) is different from equation (12) of Howard by multiplying $(\rho+p)^2$, the difference will be eliminated by boundary conditions.

3. The difference equations of Prasad and Lele

In this section, the author shows that another kind of difference equations can be obtained by the use of **Q** matrix of matrix intensity equation of Allegra and that the difference equation is the same as that of Prasad & Lele (1971), although their derivation of the equation was more complicated than that of ours.

In general, **P** matrix is a transition probability matrix. The states (complexions) defining the **P** matrix of Kakinoki and Komura and many other investigators are represented by the kinds of layers. Our states are represented by displacement vectors of layer origins parallel to layer planes, that is, the three states *AB*, *BC* and *CA* are represented by a state $\boldsymbol{d}_1 = (2/3)\boldsymbol{a}+(1/3)\boldsymbol{b}$.

The author's methods of defining states (Takahashi (1976)) are different for those of growth stacking faults, which change the sequence of layers to that of twin of original structures, and for those of deformation stacking faults. For the cases of deformation stacking faults, states are defined by the kinds of displacement vectors which are distinguished by the positions in fault free ordered structures and by fault probabilities.

Our ij element of **Q** matrix is given by the product of ij element of **P** matrix and $\varepsilon_j=\exp\{-2\pi i(\boldsymbol{s}-\boldsymbol{s}_0)(\boldsymbol{d}_j+\boldsymbol{c})/\lambda\}$ where $\boldsymbol{d}_j$ is the displacement parallel to layer planes of layer origin of the last layer of ith state to that of jth state and $\boldsymbol{c}$ is the displacement vertical to layer planes of the layer origin of the last layer of the ith state to that of the jth state.

Matrix intensity equation for close-packed structures can be rewritten by the use of our **F** and **Q** matrices by

$$I(\phi) = NV_0V_0^*\left\{1+\sum_{m=1}^{N-1}\left(1-\frac{m}{N}\right)\text{spur } \mathbf{FQ}^m \exp(-im\phi)+\text{con}j.\right\}, \tag{9}$$

where N is the number of layers and V_0 is the structure factor of layers.

Since

$$(\mathbf{FQ}^m)_{ij} = (\mathbf{FQ}^m)_{kj} \quad \text{for any } i \text{ and } k, \tag{10}$$

rewriting

$$(\mathbf{FQ}^{m-1})_{ij}=J(m, j) \quad \text{for any } i, \tag{11}$$

we can express $(\mathbf{FQ}^{m-1})_{jj}$ by a type of difference equation

$$\begin{aligned}(\mathbf{FQ}^{m-1})_{jj} &= J(m, j) \\ &= \sum_k (\mathbf{FQ}^{m-2})_{jk}Q_{kj}\end{aligned} \tag{12}$$

$$= \sum_k J(m-1, k) Q_{kj}$$
$$= \sum_k J(m-1, k) P_{kj} \varepsilon_j ,$$

that is,

$$J(m, j) = \sum_i J(m-1, i) P_{ij} \varepsilon_j . \tag{13}$$

We obtain the same number of the difference equations as that of the dimension of **Q** matrix. If two rows of **P** matrix are equal to each other, the corresponding two rows of our **Q** matrix become equal to each other. Hence, we can reduce the number of the simultaneous difference equations of this type by the same procedure as that of reduction of the number of the equations of ordinary type of the difference equations.

Although Prasad and Lele's derivation of their difference equations is very difficult to follow, their difference equations can be derived easily from equation (13). The following example shows that our and their methods give quite the same results.

Example 2.

For this example, we describe the method obtaining the difference equations for extrinsic-4c faults of d.h.c.p. discussed by Prasad & Lele (1971).

The complexions and the probability trees are given in Fig. 1. The complexions are numbered as follows,

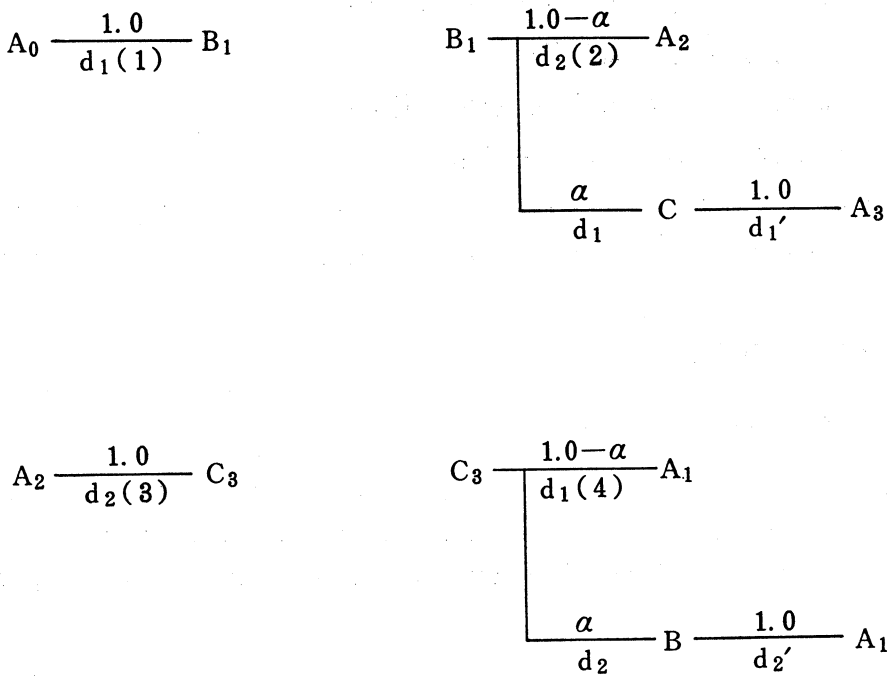

Fig. 1. Probabilities P_{ij}, complexions (states) and probability tree for extrinsic-4c faults in d.h.c.p. structures.

$$\boldsymbol{d}_1(1)=1,\quad \boldsymbol{d}_2(2)=2,\quad \boldsymbol{d}_2(3)=3,\quad \boldsymbol{d}_1(4)=4,$$

$$\boldsymbol{d}_1=5,\qquad \boldsymbol{d}_2=6,\qquad \boldsymbol{d}_1'=7,\qquad \boldsymbol{d}_2'=8.$$

The elements of **Q** are given by

$$\begin{aligned}
\boldsymbol{Q}_{12}&=\boldsymbol{Q}_{82}=(1-\alpha)\varepsilon_2,\\
\boldsymbol{Q}_{15}&=\boldsymbol{Q}_{85}=\alpha\varepsilon_1,\\
\boldsymbol{Q}_{23}&=\boldsymbol{Q}_{68}=\varepsilon_2,\\
\boldsymbol{Q}_{34}&=\boldsymbol{Q}_{74}=(1-\alpha)\varepsilon_1,\\
\boldsymbol{Q}_{36}&=\boldsymbol{Q}_{76}=\alpha\varepsilon_2,\\
\boldsymbol{Q}_{41}&=\boldsymbol{Q}_{57}=\varepsilon_1,
\end{aligned}$$

where $\varepsilon_1=\exp(2\pi i/3)$ and $\varepsilon_2=\varepsilon_1^*$. We obtain the following simultaneous difference equations by transforming **Q** so as to the 7th and 8th rows become zero,

$$\begin{aligned}
J(m,1)&=J(m-1,4)\varepsilon_1+J(m-1,6)\varepsilon_2,\\
J(m,2)&=J(m-1,1)(1-\alpha)\varepsilon_2,\\
J(m,3)&=J(m-1,2)\varepsilon_2+J(m-1,5)\varepsilon_1,\\
J(m,4)&=J(m-1,3)(1-\alpha)\varepsilon_1,\\
J(m,5)&=J(m-1,1)\alpha\varepsilon_1,\\
J(m,6)&=J(m-1,3)\alpha\varepsilon_2.
\end{aligned}$$

Hence, we have

$$\begin{aligned}
J(m,1)&=J(m-1,4)\varepsilon_1+J(m-2,3)\alpha\varepsilon_1,\\
J(m,2)&=J(m-1,1)(1-\alpha)\varepsilon_2,\\
J(m,3)&=J(m-1,2)\varepsilon_2+J(m-2,1)\alpha\varepsilon_2,\\
J(m,4)&=J(m-1,3)(1-\alpha)\varepsilon_1.
\end{aligned}$$

These equations are the same as the difference equations (23), (24), (25) and (22) of Prasad & Lele (1971) by putting $\alpha_{4c}=\alpha, \omega=\varepsilon_1$ and the other quantities $\alpha_i=0$.

4. Methods of calculations

a. Coefficients of characteristic equation

For our intensity calculation, we must obtain characteristic equation of **Q** matrix. The coefficients of the characteristic equation can be numerically calculated from Newton's formula. When the characteristic equation of **Q** is expressed by

$$a_0\rho^n+a_1\rho^{n-1}+\cdots\cdots+a_n=0, \tag{14}$$

the coefficients of characteristic equation, a_i, can be obtained from the following relations,

$$s_i = \mathrm{spur} Q^i, \tag{15a}$$

$$d_0 = a_0 = 1, \tag{15b}$$

$$d_j = (\sum_{i=1}^{j}(-1)^{i+1} d_{j-i} s_i)/j, \tag{15c}$$

$$a_j = (-1)^j d_j. \tag{15d}$$

b. Solutions of characteristic equation

We can solve numerically higher order algebraic equation by *Jarratt-modify* method. However, all the solutions obtained by this method do not necessarily satisfy the equation. Some of the solutions are not correct solutions.

When the equation is given by

$$f(x) = a_0 x^n + a_1 x^{n-1} + \cdots\cdots + a_n = 0, \tag{16}$$

if x_k is a solution, the equation can be reduced to lower order equation $g(x)$,

$$f(x) = (x - x_k) g(x), \tag{17}$$

$$g(x) = b_0 x^{n-1} + b_1 x^{n-2} + \cdots\cdots + b_{n-1}, \tag{18}$$

where $a_0 = b_0 = 1$. The coefficients b_i should satisfy

$$b_i = a_i + x_k b_{i-1}. \tag{19}$$

If the number of correct solutions are m, the order of the equation can be reduced to $n-m$. We apply the *Jarratt-modify* method to the reduced equation, and we can obtain further correct solutions. Thus, applying successively the *Jarratt-modify* method, we can obtain all the correct solutions.

c. Calculation of coefficients C_i

In this paper, we discuss only diffraction effects, so that we put the structure factor to be unity.

When the characteristic values of $\mathbf{Q}$ are $\rho_i \neq 0, i = 1, 2, \ldots, n$, where n is the dimension of $\mathbf{Q}$, $\mathrm{squr}\mathbf{FQ}^m$ is given by a linear combination of $\rho_i{}^m$,

$$\mathrm{spur}\ \mathbf{FQ}^m = \sum_{i=1}^{n} C_i \rho_i{}^m, \tag{20}$$

If all ρ_i are different to each other, the coefficients C_i can be obtained from simultaneous equations of (20) for $m = 0, 1, \ldots, n$-1. Characteristic equation of our $\mathbf{Q}$ matrix has sometimes null solutions. Equation (20) is not satisfied if the null solutions are removed in the case of $m = 0$. If we do not remove the null solutions, the linear equations for the coefficients C_i can not be solved numerically by computer since the determinant of the coefficient matrix for C_i is zero. In this case, if the number or null solutions is r, we remove the null solution from equation (20)

$$\mathrm{spur}\mathbf{FQ}^m = \sum_{i=1}^{n-r} C_i \rho_i^m, \tag{21}$$

and solve the linear equations obtained by putting m from 1 to $n-r$. Formula of Lele (1980) for C_i is suitable for the case of all solutions being not zero.

5. Diffraction effects

a. Intensity distribution

When characteristic values $\rho_i, i = 1,\ldots\ldots, n-r$, are not zero, and $\rho_i, i=n-r+1, \ldots., n$, are zero, X-ray diffracted intensity from a crystal consisting of infinite number of layers can be expressed by

$$I(\phi) = 1-2\mathrm{Re}\left(\sum_{i=1}^{n-r} C_i\right)+2\mathrm{Re}\left(\sum_{i=1}^{n-r}\sum_{m=0} C_i\rho_i^m\right) \tag{22}$$

$$= 1-2\mathrm{Re}\left(\sum_{i=1}^{n-r} C_i\right)+2\mathrm{Re}\left(\sum_{i=1}^{n-r} C_i/(1-\rho_i)\right),$$

where $\mathrm{Re}(x)$ means the real part of x.

Taking into account that $I(\phi)$ becomes large near θ_i, where $\rho_i = r_i\exp\{\mathrm{i}(\theta_i-\phi)\}$ and practically zero in the other regions, we can represent $I(\phi)$ near $\phi = \theta_i$ by $I_i(\phi)$,

$$I_i(\phi) = 2\mathrm{Re}\left(C_i\sum_{m=0}^{\infty}\rho_i^m\right)-\mathrm{Re}(C_i) \tag{23}$$

$$=2\mathrm{Re}\{C_i/(1-\rho_i)\}-\mathrm{Re}(C_i).$$

b. Integrated intensity

Integrated intensity of ith peak is defined by

$$I_i = \int_{-\pi}^{\pi} I_i(\phi)d\phi. \tag{24}$$

The integrated intensity is easily estimated by integrating equation (23) term by term and becomes

$$I_i = 2\pi\mathrm{Re}(C_i)\,. \tag{25}$$

This result agrees with that of Lele (1980).

c. Intensity maximum position

Position of maximum intensity is obtained by differentiating equation (23) and putting the result zero. The position of maximum intensity, ϕ_{im}, of ith peak is given by

$$\tan\alpha_i = \{(1+r_i^2)/(1-r_i^2)\}\tan\chi_i\,, \tag{26}$$

$$\sin(\theta_i - \phi_{im}+\alpha_i)=2r_i\sin\chi_i/\sqrt{1-2r_i^2\cos2\chi_i+r_i^4}\,, \tag{27}$$

where χ_i is defined by

$$C_i = C_{i0}\exp(i\chi_i)\,. \tag{28}$$

The intensity at ϕ_{im}, the maximum intensity, is expressed by $I(\phi_{im})$.

d. Integral breadth

Integral breadth, B_i, of the ith peak is defined by

$$\begin{aligned} B_i &= \int_{-\pi}^{\pi} I_i(\phi)d\phi / I(\phi_{im}) \\ &= 2\pi \mathrm{Re}(C_i)/I(\phi_{im})\,. \end{aligned} \tag{29}$$

e. Center of gravity of intensity distribution

Center of gravity, ϕ_{ig}, of the intensity distribution of the ith peak is defined by

$$\begin{aligned} \int_{-\pi}^{\pi} I_i(\phi)\phi d\phi &= \phi_{ig} I_i \\ &= 2\pi\phi_{ig}\mathrm{Re}(C_i)\,. \end{aligned} \tag{30}$$

The integration of the left hand side of equation (30) becomes

$$\begin{aligned} \int_{-\pi}^{\pi} I_i(\phi)\phi d\phi = {} & 2\pi \mathrm{Im}(C_i)\ln(1+2r_i\cos\theta_i + r_i^2) \\ & + 4\pi \mathrm{Re}(C_i)\tan^{-1}\{r_i\sin\theta_i/(1+r_i\cos\theta_i)\}\,, \end{aligned} \tag{31}$$

where $\mathrm{Im}(x)$ means the imaginary part of x. Hence, ϕ_{ig} is given by

$$\phi_{ig} = \ln(1+2r_i\cos\theta_i + r_i^2)\mathrm{Im}(C_i)/\mathrm{Re}(C_i) + \tan^{-1}\{r_i\sin\theta_i/(1+r_i\cos\theta_i)\}\,. \tag{32}$$

Example 3. Extrinsic-4c faults in d.h.c.p. structure

The **Q** matrix is given in example 2. The dimension of **Q** is eight, and there are four null solutions. We put the faults probability $\alpha_{4c} = 0.1$ for our numerical calculation. The coefficients of the characteristic equation are

$$a_0 = 1.0, \quad a_4 = -0.73.$$

The characteristic values are

$$\rho_1 = 0.9243378, \quad \rho_2 = -\rho_1, \rho_3 = i\rho_1, \rho_4 = -\rho_3\,.$$

The coefficients C_i obtained by using equation (21) are

$$C_1 = 0.0524935, \qquad C_2 = 0.4685723$$

$$C_3 = 0.1932342 + 0.0624245\,i\,, \quad C_4 = C_3^*.$$

The above values do not satisfy $\sum_{i-1}^{4}\mathrm{Re}(C_i) = 1$. However, the diffracted intensity calculated by equation (22) with these values exactly agrees with that calculated by equation (45) of Kakinoki & Komura (1965). When we remove the null solutions, and the range of m is taken from 0 to 3, the coefficients C_i become

$C_1 = 0.07561$ $C_2 = 0.4916887$

$C_3 = 0.2163207 + 0.0624245\,\mathrm{i}$, $C_4 = C_3^*$.

These values agree with those obtained by equation (33) of Lele (1980). From these values, we obtain for $m = 4$ the value in the left hand side of equation (21) being 0.6625 and that in the right hand side being 0.73. It is better to apply the following equation to obtain the coefficients C_1 instead of equation (33) of Lele,

$$C_1 = \sum_{i=1}^{n-r}\left(\sum_{j=1}^{i} J_j a_{i-j}\right)\rho^{n-r-i}/\rho_1 \sum_{i=1}^{n-r}\left(n-r-i+1\right)a_{i-1}\rho_1^{n-r-i}, \tag{33}$$

where $J_m = \mathrm{spur}\mathbf{FQ}^m$. The integrated intensities I_i are

$I_1 = 0.32986$, $I_2 = 2.944127$, $I_3 = 1.214126$, $I_4 = I_3$.

The intensity maximum positions ϕ_{im} are

$\phi_{1m} = 0.0$, $\phi_{2m} = 3.145927$, $\phi_{3m} = 1.58318$, $\phi_{4m} = \phi_{3m}$.

The positions of the 3rd and 4th peaks shift a little from $\pm\pi/2$. The maximum intensities $I(\phi_{im})$ are

$I(\phi_{1m}) = 1.335082$, $I(\phi_{2m}) = 11.917330$, $I(\phi_{3m}) = 5.039429$, $I(\phi_{4m}) = I(\phi_{3m})$.

The integral breadths B_i are

$B_1 = 0.247046$, $B_2 = B_1$, $B_3 = 0.240925$, $B_4 = B_3$.

The centers of gravity of the peaks ϕ_{ig} are

$\phi_{1g} = 0.0$, $\phi_{2g} = \phi_{1g}$, $\phi_{3g} = 1.691704$, $\phi_{4g} = -\phi_{3g}$.

The 1st and 2nd peaks are centro-symmetrical, and the 3rd and 4th peaks tail to larger absolute value of ϕ.

6. Remarks

Our procedure to calculate the intensity is as follows. At first, the probability tree is drawn by the method of Takahashi (1976). From the probability tree, **P** and **Q** matrices are obtained. We input **P** matrix. **F** matrix is computed from **P** matrix. **Q** matrix is also computed by multiplying column matrices of **P** by phase factors. The characteristic equation and its solutions are computed by the method described. In this case, it should be taken note of equation (22), since there are null solutions in many cases. At last, the diffraction effects are computed by the equations in the section 6. The merit of our method is to describe quantitatively the informations about each peaks.

When the equation of Kakinoki and Komura is used in our method, obtaining **P** matrix is somewhat more troublesome, since probability tree for the equation is more complex, and we must input **V** matrix. In addition, it is convinient to reduce

the matrices before input of data, although our method is not necessary to reduce matrices. The other procedures are the same as those in the case of Allegra's equation.

Since we can not know the existence of null solutions in addition to the solutions of characteristic equation of difference equation, it should occur to make error in calculation of the intensity by neglecting the null solutions. In fact, if we calculate the intensity for *Example 3* by equation (33) of Lele (1980), the result does not agree with our result which exactly agrees with that obtained by Kakinoki and Komura's method.

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