Treatment of Matrix Intensity Equation of Diffraction for Close-Packed Structures with Stacking Faults

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Synopsis

Methods obtaining continuing probabilities, with whose values the diffracted intensities can be calculated, of Allegra's intensity equation of *X*-ray diffraction for one-dimensionally disordered structures are discussed about (a) growth faults, (b) deformation faults, (c) growth and deformation faults and (d) multiple deformation faults in various close-packed structures.

1. Introduction

X-ray reflected intensities from disordered close-packed structures can be calculated either by the use of difference equation introduced by Wilson[1] or by matrix intensity equation introduced by Hendricks and Teller.[2] The treatment of the matrix intensity equation was developed by Kakinoki and Komura[3–6] and Kakinoki.[7] Allegra[8] showed that the order of the matrices of the intensity equation can be reduced if the complexions of layers are represented by the corresponding complexions of displacement vectors. Gevers[9–11] introduced a method of calculating the reflected intensities from disordered close-packed structures without solving the characteristic equations of the difference equations. His method was applied to calculation of reflected intensities by the matrix intensity equation by Kakinoki and Komura.[6] Summarizing studies of disordered f.c.c. and h.c.p. structures, Sato[12] proposed a general theory for the diffraction line profile of h.c.p. and f.c.c. polycrystals containing stacking faults.

We can calculate the reflected intensities from many kinds of disordered close-packed structures according to the procedure proposed by Kakinoki,[7] if we can know the elements of **Q** matrix, which are continuing probabilities multiplied by phase factor $e^{-i\varphi}$. However, as seen from Sato,[12] the continuing probabilities for disordered complicated structures cannot obtained straightforwardly from the original definition of Kakinoki and Komura.[3] He defined the kinds of layers by the relation to the subsequent

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layers in the cases of deformation stacking faults.

In this article, we describe the methods obtaining systematically elements of **Q** matrix of Allegra's equation for more complicated structures than f.c.c. and h.c.p. structures.

2. Intensity equation

According to Kakinoki and Komura,[6] the intensity equation in matrix form for one-dimensionally disordered structures is given by

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

The notation in equation (1) is as follows:

N is the number of layers;

$\varphi=2\pi\zeta$;

$(\boldsymbol{s}-\boldsymbol{s}_0)/\lambda=\xi\boldsymbol{a}^*+\eta\boldsymbol{b}^*+\zeta\boldsymbol{c}^*$ (scattering vector);

$\boldsymbol{s}_0$ and $\boldsymbol{s}$ are unit vectors along the incident and the scattered directions, respectively;

$\boldsymbol{a}$ and $\boldsymbol{b}$ lie in the layer and $\boldsymbol{c}$ is normal to it;

conj. means the complex conjugate of the foregoing term;

and **V**, **F** and **Q** are such matrices as

$$\left.\begin{aligned}&(\mathbf{V})_{ji}=V_iV_j^* \text{ and } (\mathbf{F})_{ij}=f_i\delta_{ij}\\&\mathbf{Q}=\mathbf{\Phi P}\\&(\mathbf{P})_{ij}=P_{ij} \text{ and } (\mathbf{\Phi})_{ij}=e^{-i\varphi_i}\delta_{ij}\\&(\mathbf{Q})_{ij}=Q_{ij}=(\mathbf{\Phi P})_{ij}=P_{ij}e^{-i\varphi_i}\end{aligned}\right\} \tag{2}$$

where

δ_{ij} is Kronecker's delta;

V_i is the layer form factor of the layer i;

f_i is the probability of finding the layer i at any position and hereafter simply called the existence probability of V_i;

P_{ij} is the probability of finding the layer j after the layer i and hereafter simply called the continuing probability of V_j after V_i;

φ_i is the phase shift due to the thickness of the layer i.

Kakinoki and Komura[4,5] made equation (1) applicable to the cases of order of

influence among layers, s, being equal to or larger than 2. In their method, a s-layer sequence is defined as a state ("a complexion of adjacent layers" according to Allegra[8]). Layer form factor of ith complexion becomes that of the last layer in the ith complexion. The elements of **F** matrix become the probabilities of finding the complexions and those of **P** matrix become the continuing probabilities of the complexions. In the case of close-packed structures, the number of complexions of adjacent layers becomes $R=3l(l=2^{s-1})$.

Since there are some number of physically equivalent complexions of adjacent layers when the layers are translatively equivalent to one another, Allegra[8] showed that dimension of the matrices in equation (1) can be reduced if a group of equivalent complexions of adjacent layers are represented by a complexion of displacement vectors and if ij element of **Q** matrix is P_{ij} multiplied by $\varepsilon_j=\exp\{-2\pi i\frac{(\boldsymbol{s}-\boldsymbol{s}_0)}{\lambda}\boldsymbol{t}_j\}$ where $\mathbf{t}_j$ is the last vector of the jth complexion of the vectors, that is, $\mathbf{Q}=\mathbf{P\Phi}$. In the case of close-packed structures, dimensions of matrices are reduced one-third and ij element of **V** matrix becomes $V_0V_0^*$, where V_0 is the layer form factor of a close-packed layer of which the origin is at the origin of the reciprocal lattice.

Since displacement vectors of close-packed structures are

$$\begin{aligned}\boldsymbol{t}_1&=\boldsymbol{d}_1+\boldsymbol{c},\ \boldsymbol{d}_1=\frac{2}{3}\boldsymbol{a}+\frac{1}{3}\boldsymbol{b},\\ \boldsymbol{t}_2&=\boldsymbol{d}_2+\boldsymbol{c},\ \boldsymbol{d}_2=\frac{1}{3}\boldsymbol{a}+\frac{2}{3}\boldsymbol{b},\end{aligned}\qquad(3)$$

equivalent layer sequences can be represented by sequences rewritten by the use of the two vectors $\boldsymbol{d}_1$ and $\boldsymbol{d}_2$. Complicated structures with long periods of layer sequence have often short periods of the vector sequences. For example, a period of *hhc* structure, *ABABCBCAC*, and its equivalences are represented by $\boldsymbol{d}_1\boldsymbol{d}_2\boldsymbol{d}_1\boldsymbol{d}_1\boldsymbol{d}_2\boldsymbol{d}_1\boldsymbol{d}_1\boldsymbol{d}_2\boldsymbol{d}_1$. A period of the vector sequence can be represented by one of the following vector sequences $\boldsymbol{d}_1\boldsymbol{d}_1\boldsymbol{d}_2$, $\boldsymbol{d}_1\boldsymbol{d}_2\boldsymbol{d}_1$ and $\boldsymbol{d}_2\boldsymbol{d}_1\boldsymbol{d}_1$.

3. Growth faults

A stacking fault is called a growth fault if it arises during crystal growth. In f.c.c. or h.c.p. structure, two parts which are bounded by a growth fault plane become twinned counterparts to each other. Kakinoki, Komura and Hiziya[13] and Kakinoki[14-16] pointed out that equivalence of a stacking sequence to its twinned counterpart should be abondoned. This type of growth faults was called "extended growth faults" by Sato.[12]

Since bond energies between layers should be quite equivalent in a structure and its twinned counterpart, we can expect the finding probabilities of the both structures to be equal to each other even in a single crystal. The difference between ordinary growth faults and extended growth faults should be practically very small. The large difference found by Kakinoki *et al* may be due to the other effect than growth faults. Since there is no difficulty in handling matrices, the growth faults in this article measn extended growth faults.

In order to formulate method obtaining continuing probabilities for growth faults in long period structures, let us take an example of growth faults in *hhc* structure. A period of vector sequence of *hhc* structure is $\boldsymbol{d}_1\boldsymbol{d}_2\boldsymbol{d}_1$. If we assume $s=3$, the complexion of vectors become:

$$(1)\ \boldsymbol{d}_1\boldsymbol{d}_2;\ (2)\ \boldsymbol{d}_2\boldsymbol{d}_1;\ (3)\ \boldsymbol{d}_1\boldsymbol{d}_1;\ (4)\ \boldsymbol{d}_2\boldsymbol{d}_2.$$

The three complexions 1, 2 and 3 are necessary to express the vector sequence in *hhc* structure. The complexion 4 arises if a stacking fault occurs after 1. If the continuing probabilities P_{12}, P_{23} and P_{31} are $1-\alpha$, then $P_{14}=P_{21}=P_{33}=\alpha$ and $P_{11}=P_{13}=P_{22}=P_{24}=P_{32}=P_{34}=0$. If P_{42} is $1-\alpha$, then $P_{44}=\alpha$ and $P_{41}=P_{43}=0$.

If $P_{42}=1-\alpha$, the vector sequence $\boldsymbol{d}_2\boldsymbol{d}_2\boldsymbol{d}_1$ should be regarded to be fault free. The structure of which the vector sequence is $\boldsymbol{d}_2\boldsymbol{d}_2\boldsymbol{d}_1\boldsymbol{d}_2\boldsymbol{d}_2\boldsymbol{d}_1\cdots$ is the twinned counterpart of the structure of which the vector sequence is $\boldsymbol{d}_1\boldsymbol{d}_1\boldsymbol{d}_2\boldsymbol{d}_1\boldsymbol{d}_1\boldsymbol{d}_2\cdots$ The continuing probability P_{23} becomes $1-\alpha>\frac{1}{2}$ for the structure of which vector sequence is $\boldsymbol{d}_1\boldsymbol{d}_1\boldsymbol{d}_2\boldsymbol{d}_1\boldsymbol{d}_1\boldsymbol{d}_2\cdots$, but becomes $\alpha'<\frac{1}{2}$ for the structure of which the vector sequence is $\boldsymbol{d}_2\boldsymbol{d}_2\boldsymbol{d}_1\boldsymbol{d}_2\boldsymbol{d}_2\boldsymbol{d}_1\cdots$ in the case $s=3$. That is, we can not uniquely define continuing probabilities in this case.

Let us denote by T the structure of which vector sequence is obtained by replacing $\boldsymbol{d}_1$ with $\boldsymbol{d}_2$ and $\boldsymbol{d}_2$ with $\mathbf{d}_1$, respectively, in the vector sequence of an ordered structure O. If the both vector sequences of O and T agree with each other, O and T belong to hexagonal system, if not, they belong to rhombohedral (or cubic) system.

There are 2^{s-1} distinct complexions which consist of s-1 vectors. The set of 2^{s-1} complexions is denoted by C. We denote by $C(O)$ and $C(T)$ the sets of the complexions which are necessary to express the **P** matrix of the ordered structures O and T, respectively. Then C is given by

$$C=C(O)+C(T)+C(c), \tag{4}$$

where $C(c)$ may or may not be null set.

If s is too small, it happens that one complexion is followed by two complexions. For example, if $s=2$, the complexion $\boldsymbol{d}_1$ is followed either by $\boldsymbol{d}_1$ or $\boldsymbol{d}_2$ in the case of *hhc* structure. Furthermore, if there are common elements between $C(O)$ and $C(T)$ in rhombohedral structures, we can not uniquely define the continuing probabilities. Hence, there is a minimum value s_0 of s, satisfying

(a) any complexion should be followed by one complexion in ordered structures,

(b) $C(O)\cap C(T)=0$ for rhombohedral structures.

For our example of *hhc* structure, s_0 becomes 4, and the complexions of vectors are:

$$(1)\ \boldsymbol{d}_1\boldsymbol{d}_1\boldsymbol{d}_2;\ (2)\ \boldsymbol{d}_1\boldsymbol{d}_2\boldsymbol{d}_1;\ (3)\ \boldsymbol{d}_2\boldsymbol{d}_1\boldsymbol{d}_1;\ (4)\ \boldsymbol{d}_1\boldsymbol{d}_1\boldsymbol{d}_1;$$
$$(5)\ \boldsymbol{d}_2\boldsymbol{d}_2\boldsymbol{d}_1;\ (6)\ \boldsymbol{d}_2\boldsymbol{d}_1\boldsymbol{d}_2;\ (7)\ \boldsymbol{d}_1\boldsymbol{d}_2\boldsymbol{d}_2;\ (8)\ \boldsymbol{d}_2\boldsymbol{d}_2\boldsymbol{d}_2;$$

and $C(O)=\{1, 2, 3\}$, $C(T)=\{5, 6, 7\}$, $C(c)=\{4, 8\}$. The continuing probabilities are:

$$P_{12}=P_{23}=P_{31}=1-\alpha;\ P_{17}=P_{26}=P_{34}=\alpha;$$
$$P_{56}=P_{67}=P_{75}=1-\alpha';\ P_{53}=P_{62}=P_{78}=\alpha';$$
$$P_{41}=1-\beta;\ P_{44}=\beta;\ P_{85}=1-\beta';\ P_{88}=\beta';$$

and the others are zero. Since the complexion 4 or 8 does not belong to $C(O)$ or $C(T)$, the probabilities β and β' may be different from α and α', respectively. If we wish to obtain more accurate intensity, we should put $P_{17}\neq P_{26}\neq P_{34}<\frac{1}{2}$ and $P_{53}\neq P_{62}\neq P_{78}<\frac{1}{2}$.

4. Deformation faults and growth and deformation faults

A deformation fault arises if a shearing force parallel to the stacking layers gives rise to a transformation of one half of the close-packed crystal relative to the other half.[12] Deformation faults are characterized by a continuance of the displacement throughout subsequent layers. For example, if a part *ACA* in the layer sequence *ABACA* is displaced, *ACA* becomes *CBC*. The vector sequence $\boldsymbol{d}_1\boldsymbol{d}_2\boldsymbol{d}_2\boldsymbol{d}_1$ for *ABACA* is changed to $\boldsymbol{d}_1\boldsymbol{d}_1\boldsymbol{d}_2\boldsymbol{d}_1$ in this case. Then, the average displacement in the second position of the vector sequence becomes $(1-\beta)\boldsymbol{d}_2+\beta\boldsymbol{d}_1$, if the probability of the occurence of the deformation fault is β. The vectors at the other positions remain unchanged.

When elements of **F** and **P** matrices for a basic (ordered or disordered) structure are given, the contribution of the X-ray interference between s and t layers to the total reflected intensity, where it is assumed that s is followed by a, b, $\cdots$, q and t layers, is given by

$$f_s P_{sa} P_{ab} \cdots P_{qt} e^{-i\varphi_a} e^{-i\varphi_b} \cdots e^{-i\varphi_t} + conj. = f_s Q_{sa} Q_{ab} \cdots Q_{qt} + conj. \quad (5)$$

If a deformation fault occurs after a, the a should be followed by b with the probability $P_{ab}(1-\beta)$ and by r, which is different from a and b, with the probability $P_{ab}\beta$. Then the contribution to the intensity becomes

$$\begin{aligned} & f_s P_{sa} P_{ab} (1-\beta) P_{bc} \cdots P_{qt} e^{-i\varphi_a} e^{-i\varphi_b} \cdots e^{-i\varphi_t} + conj. \\ & \quad + f_s P_{sa} P_{ab} \beta P_{bc} \cdots P_{qt} e^{-i\varphi_a} e^{-i\varphi_r} \cdots e^{-i\varphi_t} + conj. \\ & = f_s Q_{sa} P_{ab} \{(1-\beta) e^{-i\varphi_b} + \beta e^{-i\varphi_r}\} Q_{bc} \cdots Q_{qt} + conj. \end{aligned} \quad (6)$$

Equation (6) is obtained by replacing $e^{-i\varphi_b}$ in equation (5) with $(1-\beta)e^{-i\varphi_b} + \beta e^{-i\varphi_r}$.

We can conclude that the intensity from a structure with deformation faults can be obtained by replacing ε_i of the $\mathbf{Q}$ matrix for the basic structure with the average value $(1-\beta)\varepsilon_i + \beta\varepsilon_j$, where $\varepsilon_i \neq \varepsilon_j$, without changing the other matrices.

Example 1. Deformation faults in *hc* structure

In general, if characteristic equations of $\mathbf{Q}' = \mathbf{Q}e^{i\varphi}$ matrices obtained by our method agree those obtained by the others, our reflected intensities should be the same with those obtained by the others. We only show the equality between our characteristic equations and those obtained by the others.

Since a period of the vector sequence of ordered *hc* structure is $\boldsymbol{d}_1\boldsymbol{d}_2\boldsymbol{d}_2\boldsymbol{d}_1$, we can put the elements of the $\mathbf{Q}$ matrix as follows:

$$Q_{12} = Q_{23} = \varepsilon_2;\ Q_{34} = Q_{41} = \varepsilon_1;$$

and all the others are zero. Hence, the elements of the $\mathbf{Q}$ matrix for the deformation faults become:

$$Q_{12} = Q_{23} = (1-\beta)\varepsilon_2 + \beta\varepsilon_1;\ Q_{34} = Q_{41} = (1-\beta)\varepsilon_1 + \beta\varepsilon_2;$$

and all the others are zero.

The characteristic equation of the $\mathbf{Q}'$ matrix is

$$x^4 - \{1 - 3(1-\beta)\beta\}^2 = 0$$

and it agrees with that obtained by Gevers.[10]

For growth and deformation faults, elements of **Q** matrix can be easily obtained. At first, we obtain **Q** matrix for growth faults, then replace the phase factor ε_i with the average value $(1-\beta)\varepsilon_i+\beta\varepsilon_j$. The **F** matrix can be obtained from **MFP**=**MF** where **P** matrix is for the growth faults and $(\mathbf{M})_{ij}=1$.

Example 2. Growth and deformation faults in h.c.p. structure

This problem was solved by Sato.[12] His complexions were defined by the kinds of layers and their relation to subsequent layers. When we put $\alpha_1=\alpha_2=\beta=0$ in his probabilities, it turns out that his basic layer sequences are $B_2A_1B_2A_1\cdots$, $C_1A_2C_1A_2\cdots$, and their cyclic equivalences. When we put $\beta=0$, the layer sequence B_2A_1 is followed by B_2 with the probability $1-\alpha_2$ and C_1A_2 is followed by C_1 with the probability $1-\alpha_1$. Since the layer sequence B_2A_1 and C_1A_2 correspond to the displacement vectors $\boldsymbol{d}_2$ and $\boldsymbol{d}_1$, respectively, we can define the complexions of vectors by (1) $\boldsymbol{d}_2$ and (2) $\boldsymbol{d}_1$, correspondingly to Sato's complexions.

Our elements of **P** matrix for growth faults become:

$$P_{11}=\alpha_2;\ P_{12}=1-\alpha_2;\ P_{21}=1-\alpha_1;\ P_{22}=\alpha_1.$$

The elements of **F** matrix are obtained as follows:

$$f_1=\frac{1-\alpha_1}{2-\alpha_1-\alpha_2}=w_1;\ f_2=\frac{1-\alpha_2}{2-\alpha_1-\alpha_2}=w_2.$$

Accordingly, the elements of **Q** matrix for the growth and deformation faults become:

$$Q_{11}=\alpha_2\{(1-\beta)\varepsilon_2+\beta\varepsilon_1\};\ Q_{12}=(1-\alpha_2)\{(1-\beta)\varepsilon_1+\beta\varepsilon_2\};$$
$$Q_{21}=(1-\alpha_1)\{(1-\beta)\varepsilon_2+\beta\varepsilon_1\};\ Q_{22}=\alpha_2\{(1-\beta)\varepsilon_1+\beta\varepsilon_2\}.$$

The **Q** matrix can be rewritten by

$$\mathbf{Q}=\varepsilon_1\mathbf{P}_1+\varepsilon_2\mathbf{P}_2.$$

Since the **Q** matrix agrees with Sato's reduced **Q** matrix and the elements of Sato's **F** matrix are $f_1=f_3=f_5=\frac{1}{3}w_1$ and $f_2=f_4=f_6=\frac{1}{3}w_2$, our intensity should agree with that of Sato.

5. Multiple deformation faults

The treatment of mutliple deformation faults in f.c.c. structure was described by

Kakinoki,[8] his method fails applicability for h.c.p. structure. This can be easily seen. According to his method, the complexions are indicated by six kinds of layers, A, B, C, A', B' and C'. The complexions A', B' and C' follow B, C and A with the probability β and are followed by C, A and B with the probability 1, respectively. In the case of double deformation, if we represent by $ABAB\cdots$ the layer sequences in h.c.p. structure, B is followed by C' and C' is followed by A, on the other hand, B is followed by C' and C' is followed by B. Hence, we can not uniquely obtain **P** matrix in this case. That is, Kakinoki's method fails applicability in the case of h.c.p. structure.

Concerning to double deformation faults in h.c.p. structure, Sato[17] calculated the diffracted intensity using quite similar complexions as those for growth and deformation faults in h.c.p. structure. Although his method is very useful to the cases of f.c.c. and h.c.p. structures, it can not be applicable to the other long period structures. For example, *hc* structure has $ABAC$ as one period of layer sequence. The layer sequence $ABAC$ can be expressed as $A_1B_2A_2C_1$ by Sato's method. The complexion A_1 is followed by C_2' with the probability β, and C_2' is followed by A_2 with the probability 1. The complexion B_2 is followed also by C_2' with the probability β, and C_2' is folloswed by A_1 with the probability 1. Hence, we can not uniquely obtain **P** matrix in this case.

If we represent layer sequences by displacement vector sequences, a deformation fault only changes the vector at the position corresponding to the fault plane and does not change the other vectors. Hence, we can indicate a complexion for an ordered structure by the displacement vectors and their positions. For exmaple, the complexions for ordered *hc* structure are:

$$(1)\ \boldsymbol{d}_1(1);\ (2)\ \boldsymbol{d}_2(2);\ (3)\ \boldsymbol{d}_2(3);\ (4)\ \boldsymbol{d}_1(4).$$

If a double deformation fault occurs after $\boldsymbol{d}_1(1)$, $\boldsymbol{d}_1(1)$ is followed by $\boldsymbol{d}_1$ with the probability β, $\boldsymbol{d}_1$ is followed by $\boldsymbol{d}_1$ with the probability 1 and finally $\boldsymbol{d}_1$ should be followed by $\boldsymbol{d}_1(4)$ with the probability $1-\beta$. If a double deformation fault occurs after $\boldsymbol{d}_2(2)$, $\boldsymbol{d}_2(2)$ is followed by $\boldsymbol{d}_1$, $\boldsymbol{d}_1$ is followed by $\boldsymbol{d}_2$ and finally $\boldsymbol{d}_2$ should be followed by $\boldsymbol{d}_1(1)$ with the probability $1-\beta$. The above example shows that we cannot distinguish the complexions by the vectors and their positions.

Complexions for the deformation faults can be indicated by the positions of the displacement vectors in the vector sequence of the ordered structure and the continuing probabilities with which the displacement vectors follow the preceding vectors.

For our example, the additional complexions necessary to express the **P** matrix become:

$$(5)\ \boldsymbol{d}_2(1)';\ (6)\ \boldsymbol{d}_1(2)';\ (7)\ \boldsymbol{d}_1(3)';\ (8)\ \boldsymbol{d}_2(4)';$$
$$(9)\ \boldsymbol{d}_2(1)'';\ (10)\ \boldsymbol{d}_1(2)'';\ (11)\ \boldsymbol{d}_1(3)'';\ (12)\ \boldsymbol{d}_2(4)''.$$

The complexion 1 is followed by 2 and 6 with the probabilities $1-\beta$ and β, respectively, 6 is followed by 11 with the probability 1 and 11 is followed by 4 and 8 with the probabilities $1-\beta$ and β, respectively.

In general, if a period of vector sequence of an ordered structure has n vectors, the number of the necessary complexions for defining **P** matrix of m-ple deformation faults becomes $n(1+m)$ in our method.

Example 3. Double deformation faults in h.c.p. structure

Our complexions are:

$$(1)\ \boldsymbol{d}_1(1);\ (2)\ \boldsymbol{d}_2(2);\ (3)\ \boldsymbol{d}_2(1)';$$
$$(4)\ \boldsymbol{d}_1(2)';\ (5)\ \boldsymbol{d}_2(1)'';\ (6)\ \boldsymbol{d}_1(2)''.$$

The elements of **P** matrix are:

$$P_{12}=P_{21}=P_{52}=P_{61}=1-\beta;\ P_{14}=P_{23}=P_{54}=P_{63}=\beta;\ P_{36}=P_{45}=1;$$

and the others are zero. The characteristic equation of **Q**′ matrix is

$$x^2[x^4-\{2\beta+(1-\beta)^2\}x^2+\beta^2]=0$$

The equation is practically identical to that of Sato.[17]

In the case of h.c.p. structure, our **Q** matrix for double deformation faults is of six dimension. The dimension of Sato's **Q** matrix is essentially four. Sato's method is better than ours in this case. However, his method cannot be developed to the other more complicated structures. In this point, our method is more general than that of Sato.

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