Simultaneous Diffraction of X-rays

Hidewo TAKAHASHI

Group-theoretical treatment of X-ray simultaneous diffraction in the symmetric Laue case is discussed by developing the theory of Kogiso and Takahashi [J. Phys, Soc. Japan, **42** (1977), 223] for electron diffraction. An application of the theory is shown by a solvable example of the four-wave case in which the little co-group of wave vector is C_{2v}.

1. Introduction

The author and his collaborator have studied application of group theory to many-beam electron diffraction.[1] This article describes development of their theory to the case of simultaneous diffraction of X-rays.[4-6]

One of the difficulties in X-ray diffraction lies in the fact that X-rays are transverse and their wave-fields are vector fields. It is necessary to define two unit polarization vectors which are perpendicular to a wave vector in order to describe the direction of vibration of the wave. The form of fundamental equations of X-ray diffraction depends on the choice of the directions of the polarization vectors and the number of the equations becomes $2n$ in the case of n-wave approximation. The symmetry of the fundamental equations of X-ray diffraction can not be seen easily in contrast to that of electron diffraction. X-rays in a crystal should be subject to the symmetry of the crystal and satisfy the boundary condition. These conditions are quite similar to those of electrons in crystal.[1] The symmetry group of a wave-field of X-rays should be also the little group of the wave vector. Fundamental equations of X-ray diffraction can be reduced if the representations of symmetry operations which transform invariantly the equations are obtained. The representations become very simple if the polarization vectors are defined in proper manner such as Joko and Fukuhara's.[6]

In this article, we discuss the symmetric Laue case where all the waves satisfy Bragg condition. The fundamental equations are rewritten as a matrix form in section 2. Polarization vectors are defined in order that they should be transformed into those of the same kind by symmetry operations and the forms of the representation of the symmetry operations are given in section 3. Reduction of matrices in the matrix form of fundamental equations is described in section 4. The method is quite similar to the case of electron diffraction.[1] Boundary conditions in our case are also given as a matrix form. Finally, an example of solution is shown in section 5 where the number of waves is four and the little co-group is C_{2v}.

2. Matrix Form of Fundamental Equations

When a plane monochromatic X-ray wave is incident over a crystal, a wave-field (electric= displacement-field) vector $\boldsymbol{D}$ in the crystal can be written as a superposition of plane waves,

$$\boldsymbol{D}=\exp(\mathrm{i}\nu t)\sum_{h}\boldsymbol{D}_h\exp(-\mathrm{i}\boldsymbol{k}_h\boldsymbol{r}), \tag{1}$$

where $\boldsymbol{k}_h=\boldsymbol{k}_0+2\pi\boldsymbol{h}$ is the wave vector of hth wave, and direction of $\boldsymbol{D}_h$ is perpendicular to $\boldsymbol{k}_h$. The component wave-field vector $\boldsymbol{D}_h$ is given by the sum of $D_h^\sigma\boldsymbol{\sigma}_h$ and $D_h^\pi\boldsymbol{\pi}_h$ where $\boldsymbol{\sigma}_h$ and $\boldsymbol{\pi}_h$ are unit polarization vectors.

The fundamental equations of X-ray diffraction are given by

$$\begin{aligned} x_hD_h^\sigma&=\sum_g{}'v_{h-g}\{(\boldsymbol{\sigma}_h\cdot\boldsymbol{\sigma}_g)D_g^\sigma+(\boldsymbol{\sigma}_h\cdot\boldsymbol{\pi}_g)D_g^\pi\}\\ x_hD_h^\pi&=\sum_g{}'v_{h-g}\{(\boldsymbol{\pi}_h\cdot\boldsymbol{\sigma}_g)D_g^\sigma+(\boldsymbol{\pi}_h\cdot\boldsymbol{\pi}_g)D_g^\pi\}\end{aligned} \tag{2}$$

where x_h is defined by the relation

$$\boldsymbol{K}^2x_h=\boldsymbol{K}^2(1-v_0)-\boldsymbol{k}_h^2, \tag{3}$$

and v_g is the gth Fourier coefficient of the polarizability of the crystal.

Equation (2) can be rewritten as a matrix form,

$$\mathsf{M}\boldsymbol{\Psi}=\mathsf{X}\boldsymbol{\Psi}, \tag{4}$$

where matrices M and X have hg submatrices

$$\mathsf{M}_{hg}=\begin{cases}\begin{pmatrix}0&0\\0&0\end{pmatrix} & \text{for}\quad h=g,\\ v_{h-g}\begin{pmatrix}(\boldsymbol{\sigma}_h\cdot\boldsymbol{\sigma}_g)&(\boldsymbol{\sigma}_h\cdot\boldsymbol{\pi}_g)\\(\boldsymbol{\pi}_h\cdot\boldsymbol{\sigma}_g)&(\boldsymbol{\pi}_h\cdot\boldsymbol{\pi}_g)\end{pmatrix} & \text{for}\quad h\neq g,\end{cases} \tag{5}$$

and

$$\mathsf{X}_{hg}=\begin{cases}x_h\begin{pmatrix}1&0\\0&1\end{pmatrix} & \text{for}\quad h=g,\\ \begin{pmatrix}0&0\\0&0\end{pmatrix} & \text{for}\quad h\neq g,\end{cases} \tag{6}$$

and a column vector $\boldsymbol{\Psi}$ has hth subvector

$$\boldsymbol{\Psi}_h=\begin{pmatrix}D_h^\sigma\\D_h^\pi\end{pmatrix}. \tag{7}$$

Equation (4) is similar to the fundamental equation of electron diffraction,[1] although

matrix elements and vector components are replaced by submatrices and subvectors of order 2. If all the waves satisfy Bragg condition, all the values of x_h become equal to one another and eq. (4) reduces to an eigenvalue problem. We can easily see that M is Hermitian for non-absorbing crystals.

3. Symmetry Representation

Similarly to the case of electron diffraction,[1] the wave vector $\boldsymbol{k}_0$ of a wave-field of X-rays in a crystal should satisfy

$$A\boldsymbol{k}_0=\boldsymbol{k}_0+2\pi\boldsymbol{H}(A) \tag{8}$$

and

$$A\boldsymbol{k}_n=\boldsymbol{k}_n, \tag{9}$$

where A is a rotation of symmetry operation of the space group of the crystal, $\boldsymbol{H}(A)$ is a reciprocal lattice vector normal to $\boldsymbol{k}_n$, and $\boldsymbol{k}_n$ is the normal component of $\boldsymbol{k}_0$ to the crystal surface. The symmetry operations satisfying eqs. (8) and (9) form a subgroup of the space group of the crystal. The subgroup is called the little group of the wave vector $\boldsymbol{k}_0$, $G(\boldsymbol{k}_0)$,[7] and the symmetry group of the wave-field.

To form the representations of $G(\boldsymbol{k}_0)$, we define bases by

$$\begin{aligned}\boldsymbol{f}_g&=[\boldsymbol{\sigma}_g\exp(-i\boldsymbol{k}_g\boldsymbol{r})\quad\boldsymbol{\pi}_g\exp(-i\boldsymbol{k}_g\boldsymbol{r})]\\&=[\boldsymbol{f}_{g\sigma}\ \ \boldsymbol{f}_{g\pi}].\end{aligned} \tag{10}$$

The transform of the base $\boldsymbol{f}_g$ is given by

$$R\boldsymbol{f}_g=[R\boldsymbol{f}_{g\sigma}\ R\boldsymbol{f}_{g\pi}], \tag{11}$$

where

$$R\boldsymbol{f}_{g\sigma}=(A\boldsymbol{\sigma}_g)\exp[-i\{\boldsymbol{k}_0+2\pi(A\boldsymbol{g}+\boldsymbol{H}(A))\}(\boldsymbol{r}-\boldsymbol{t})] \tag{12}$$

and

$$R\boldsymbol{f}_{g\pi}=(A\boldsymbol{\pi}_g)\exp[-i\{\boldsymbol{k}_0+2\pi(A\boldsymbol{g}+\boldsymbol{H}(A))\}(\boldsymbol{r}-\boldsymbol{t})]. \tag{13}$$

In general, $A\boldsymbol{\sigma}_g$ and $A\boldsymbol{\pi}_g$ are given by linear combinations of $\boldsymbol{\sigma}_{Ag+H(A)}$ and $\boldsymbol{\pi}_{Ag+H(A)}$. We define a row vector $\boldsymbol{F}$ by

$$\boldsymbol{F}=[\boldsymbol{f}_0\cdots\boldsymbol{f}_g\cdots\boldsymbol{f}_h\cdots]. \tag{14}$$

Unit polarization vectors $\boldsymbol{\sigma}_g$ and $\boldsymbol{\pi}_g$ are defined by

$$\boldsymbol{\sigma}_g=\frac{\boldsymbol{k}_g\times\boldsymbol{K}_n}{|\boldsymbol{k}_g\times\boldsymbol{K}_n|} \tag{15}$$

and

$$\boldsymbol{\pi}_g = \frac{\boldsymbol{k}_g \times \boldsymbol{\sigma}_g}{|\boldsymbol{k}_g \times \boldsymbol{\sigma}_g|}, \tag{16}$$

where $\boldsymbol{K}_n$ is the normal component of $\boldsymbol{K}$, the incident wave vector in vacuum, to the crystal surface.[6] Then, we have

$$A\boldsymbol{\sigma}_g = |A|\boldsymbol{\sigma}_{Ag+H(A)} \tag{17}$$

and

$$A\boldsymbol{\pi}_g = \boldsymbol{\pi}_{Ag+H(A)}, \tag{18}$$

where $|A|=1$ for proper rotations and $|A|=-1$ for improper rotations.

The representation $\mathsf{D}(R)$ of a symmetry operation R is defined by

$$R\boldsymbol{f}_g = \sum_h \boldsymbol{f}_h D(R)_{hg}. \tag{19}$$

From eqs. (12), (13), (17), (18) and (19), each of element of the representation of $R=\{A|\boldsymbol{t}\}$ becomes

$$D(R)_{hg} = \begin{pmatrix} D(R)_{hg}^{(\sigma)} & 0 \\ 0 & D(R)_{hg}^{(\pi)} \end{pmatrix} \tag{20}$$

$$= \begin{pmatrix} |A| & 0 \\ 0 & 1 \end{pmatrix} \exp(-\mathrm{i}\boldsymbol{k}_h\boldsymbol{t})\delta_{h,Ag+H(A)}.$$

4. Reduction of Fundamental Equations

The representation $\mathsf{D}(R)$ can be reduced into a direct sum of irreducible representations (*reps*) $\mathsf{D}^{(\lambda)}(R)$ of $G(\boldsymbol{k}_0)$,[1]

$$\mathsf{T}^{-1}\mathsf{D}(R)\mathsf{T} = \sum_\lambda n(\lambda)\mathsf{D}^{(\lambda)}(R), \tag{21}$$

where T is a similarity transformation matrix. The values of $n(\lambda)$ are given by

$$n(\lambda) = \frac{1}{|G|}\sum_R \chi^{(\lambda)}(R)^*\chi(R), \tag{22}$$

where $|G|$ is the order of $G(\boldsymbol{k}_0)$, and $\chi^{(\lambda)}(R)$ and $\chi(R)$ are the characters of $\mathsf{D}^{(\lambda)}(R)$ and $\mathsf{D}(R)$, respectively. Furthermore, since $\mathsf{D}(R)$ can be rewritten by a block-diagonal form

$$\dot{\mathsf{D}}(R) = \mathsf{D}(R)^{(\sigma)} + D(R)^{(\pi)}, \tag{23}$$

$n(\lambda)$ becomes

$$n(\lambda) = n(\lambda, \sigma) + n(\lambda, \pi), \tag{24}$$

where

$$n(\lambda, \alpha)=\frac{1}{|G|}\sum_{R}\chi^{(\lambda)}(R)^{*}\chi(R)^{(\alpha)} \tag{25}$$

and $\chi(R)^{(\alpha)}$ is the character of $\mathsf{D}(R)^{(\alpha)}$ for $\alpha=\sigma, \pi$.

We can generate symmetry-adapted bases ϕ_t, $t=1,\ldots, i(\lambda)$, for the λ *rep* from a base $\boldsymbol{f}$ by

$$\begin{aligned}\phi_t &= W_{ts}\boldsymbol{f} \\ &= \frac{i(\lambda)}{|G|}\sum_{R}D^{(\lambda)}(R)^{*}_{ts}R\boldsymbol{f},\end{aligned} \tag{26}$$

if $W_{ss}\boldsymbol{f}\neq 0$, where $i(\lambda)$ is the dimension of the λ *rep*. Since symmetrically equivalent bases generate equivalent systems of symmetry-adapted bases for the same s, we can choose $\boldsymbol{f}_{0\sigma}$ and $\boldsymbol{f}_{0\pi}$ as the generating bases if all waves satisfy Bragg condition and they are symmetrically equivalent with one another. The $2n$ symmetry-adapted functions can be labelled as $\phi^{(\lambda in)}$, where $\lambda=\alpha,\ldots, \nu$, $n=1,\ldots, n(\lambda)$ and $i=1,\ldots, i(\lambda)$. We define row vectors by

$$\boldsymbol{S}^{(\lambda n)}=[\phi^{(\lambda 1 n)}\phi^{(\lambda 2 n)}\cdots\phi^{(\lambda i(\lambda) n)}] \tag{27}$$

and

$$\boldsymbol{S}=[\boldsymbol{S}^{(\alpha 1)}\cdots\boldsymbol{S}^{(\alpha n(\alpha))}\cdots\boldsymbol{S}^{(\nu n(\nu))}]\,. \tag{28}$$

The similarity transformation matrix T satisfying eq. (21) is obtained by

$$\boldsymbol{S}=\boldsymbol{F}\mathsf{T}. \tag{29}$$

The matrix T has the same properties as T of eq. (3.6) of Kogiso and Takahashi.[1)]

In quite the same way as in electron diffraction,[1)] M can be reduced by T to the block-diagonal form where diagonal submatrices have $i(\lambda)n(\lambda)$ dimension,

$$\mathsf{T}^{-1}\mathsf{M}\mathsf{T}=\bar{\mathsf{M}}=\sum_{\lambda}\mathsf{M}^{(\lambda)}. \tag{30}$$

As we will show in the later section, we can more easily solve the fundamental equations (2) by substituting of suitable linear combinations of symmetry-adapted bases to eq. (2) than by reducing the matrix M to the form of $\bar{\bar{\mathsf{M}}}$ in the case of electron diffraction.[1)] Our discussion in this section is for the theoretical ground of solving eq. (2).

Equation (4) is transformed by T,

$$\bar{\mathsf{M}}(\mathsf{T}^{-1}\boldsymbol{\Psi})=x(\mathsf{T}^{-1}\boldsymbol{\Psi}) \tag{31}$$

The eigenvalues and eigenvectors of eq. (31) are obtained by solving reduced eigenvalue problems

$$\mathsf{M}^{(\lambda)}\boldsymbol{a}=x\boldsymbol{a}, \tag{32}$$

for $\lambda=\alpha,\ldots, \nu$. If $\boldsymbol{a}^{(\lambda i)}$ is ith eigenvector belonging to λ *rep* of eq. (32), the corresponding eigenvector $\boldsymbol{A}^{(\lambda i)}$ of eq. (31), where $\boldsymbol{A}=\mathsf{T}^{-1}\boldsymbol{\Psi}$, satisfies

$$\bar{\mathsf{M}}\boldsymbol{A}^{(\lambda i)}=\mathsf{M}^{(\lambda)}\boldsymbol{a}^{(\lambda i)}. \tag{33}$$

If T is orthogonal and $\boldsymbol{A}^{(\lambda i)}$s are orthonormalized, the eigenvectors $\boldsymbol{\Psi}$s are orthonormalized.

In addition to tangential continuity of wave vectors, the wave-field vectors should satisfy

$$\sum_{j=1}^{2n}\boldsymbol{D}_h^{(j)}=\boldsymbol{D}_0^{(e)}\delta_{h0}, \tag{34}$$

where j, corresponding to the above (λi), indicates the branch number of dispersion surface and $\boldsymbol{D}_0^{(e)}$ is the electric displacement of the incident wave in vacuum.[4]

Since $\boldsymbol{D}_0^{(e)}$ can be expressed as $\boldsymbol{\sigma}_0\cos\gamma+\boldsymbol{\pi}_0\sin\gamma$, the boundary conditions can be written by

$$\sum_{j=1}^{2n}c_j\begin{pmatrix}\Psi_{h\sigma}^{(j)}\\ \Psi_{h\pi}^{(j)}\end{pmatrix}=\begin{pmatrix}\cos\gamma\\ \sin\gamma\end{pmatrix}\delta_{h0}, \tag{35}$$

where $\Psi_{h\sigma}^{(j)}$ and $\Psi_{h\pi}^{(j)}$ are the elements of jth eigenvector $\boldsymbol{\Psi}^{(j)}$, and γ is the angle between $\boldsymbol{\sigma}_0$ and $\boldsymbol{D}_0^{(e)}$. From orthonormality of $\boldsymbol{\Psi}^{(j)}$s, c_j turns out to be

$$c_j=\Psi_{0\sigma}^{(j)*}\cos\gamma+\Psi_{0\pi}^{(j)*}\sin\gamma. \tag{36}$$

Then, we have

$$\boldsymbol{D}_h^{(j)}=c_j(\Psi_{h\sigma}^{(j)}\boldsymbol{\sigma}_h+\Psi_{h\pi}^{(j)}\boldsymbol{\pi}_h)\,. \tag{37}$$

5. Example of Application

Joko and Fukuhara[6] listed solvable arrangements of reciprocal lattice points in which eigenvalue equations can be reduced to quadratic equations, and showed the eigenvalues and eigenvectors. Besides, when a crystal class is symmorphic, the little co-group is C_{2v} and four reciprocal lattice points lie exactly on the Ewald sphere, the eigenvalue equations can be reduced also to four quadratic equations. This is another solvable case.

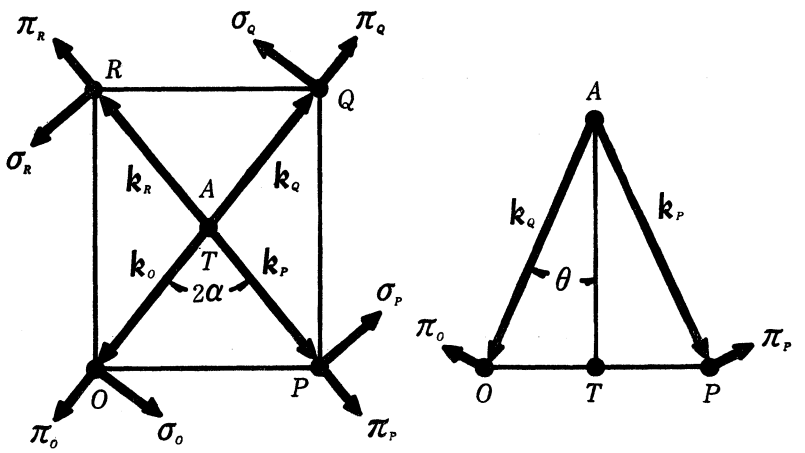

Fig. 1. Arrangement of reciprocal lattice points and directions of unit polarization vectors $\boldsymbol{\sigma}_h$ and $\boldsymbol{\pi}_h$.
$2\alpha=\angle OTP$, $2\theta=\angle OAQ$.

The arrangement of reciprocal lattice points and directions of unit polarization vectors $\boldsymbol{\sigma}_h$ and $\boldsymbol{\pi}_h$ are shown in Fig. 1. This case was recently studied by Post et al.[8] In their study the crystal system is cubic and the reciprocal lattice points O, P, Q and R have the indices 000, $1\bar{1}1$, $3\bar{1}\bar{1}$ and $20\bar{2}$, respectively.

By putting $v_P=a$, $v_Q=b$ and $v_R=c$, the matrix M becomes

$$\mathsf{M}=\begin{bmatrix} 0 & a\mathsf{V}_1 & b\mathsf{V}_2 & c\mathsf{V}_3 \\ a\tilde{\mathsf{V}}_1 & 0 & c\tilde{\mathsf{V}}_3 & b\mathsf{V}_2 \\ b\mathsf{V}_2 & c\mathsf{V}_3 & 0 & a\mathsf{V}_1 \\ c\tilde{\mathsf{V}}_3 & b\mathsf{V}_2 & a\tilde{\mathsf{V}}_1 & 0 \end{bmatrix} \tag{38}$$

where $\mathsf{V}_1=\begin{pmatrix} A & B \\ -B & C \end{pmatrix}$, $\mathsf{V}_2=\begin{pmatrix} -1 & 0 \\ 0 & D \end{pmatrix}$, $\mathsf{V}_3=\begin{pmatrix} -A & -B \\ B & E \end{pmatrix}$, $A=\cos 2\alpha$, $B=\cos\theta\sin 2\alpha$, $C=1-2\cos^2\theta\sin^2\alpha$, $D=-\cos 2\theta$, $E=1-2\cos^2\theta\cos^2\alpha$, $\tilde{\mathsf{V}}_1$ and $\tilde{\mathsf{V}}_3$ are the transposed matrices of V_1 and V_3. Since the directions of our unit polarization vectors $\boldsymbol{\sigma}_h$ and $\boldsymbol{\pi}_h$ are defined by different principle from those of Post et al.,[8] we can not simply relate the elements of M with eq. (8) of them.

The *reps* of C_{2v} are all one-dimensional and denoted by A_1, A_2, B_1 and B_2. The characters of the *reps* are shown in Table I. All the values of $n(\lambda, \sigma)$ and $n(\lambda, \pi)$ become equal to unity, i.e. all the values of $n(\lambda)$ are equal to two. Symmetry-adapted bases in

Table I. Character table of C_{2v}.

	E	$C_2(z)$	m_1	m_2
A_1	1	1	1	1
A_2	1	1	−1	−1
B_1	1	−1	1	−1
B_2	1	−1	−1	1

Table II. Elements of T.

	λ	A_1		A_2		B_1		B_2	
	α	σ	π	σ	π	σ	π	σ	π
g	j	1	2	1	2	1	2	1	2
O	σ	$\frac{1}{2}$	0	$\frac{1}{2}$	0	$\frac{1}{2}$	0	$\frac{1}{2}$	0
	π	0	$\frac{1}{2}$	0	$\frac{1}{2}$	0	$\frac{1}{2}$	0	$\frac{1}{2}$
P	σ	$-\frac{1}{2}$	0	$\frac{1}{2}$	0	$\frac{1}{2}$	0	$-\frac{1}{2}$	0
	π	0	$\frac{1}{2}$	0	$-\frac{1}{2}$	0	$-\frac{1}{2}$	0	$\frac{1}{2}$
Q	σ	$\frac{1}{2}$	0	$\frac{1}{2}$	0	$-\frac{1}{2}$	0	$-\frac{1}{2}$	0
	π	0	$\frac{1}{2}$	0	$\frac{1}{2}$	0	$-\frac{1}{2}$	0	$-\frac{1}{2}$
R	σ	$-\frac{1}{2}$	0	$\frac{1}{2}$	0	$-\frac{1}{2}$	0	$\frac{1}{2}$	0
	π	0	$\frac{1}{2}$	0	$-\frac{1}{2}$	0	$\frac{1}{2}$	0	$-\frac{1}{2}$

eq. (26) are produced by $\boldsymbol{f}_{0\sigma}$ and $\boldsymbol{f}_{0\pi}$ and elements of T are given in Table II.

If two symmetry-adapted bases belonging to λ *rep* are denoted by $\phi^{(\lambda 1)}$ and $\phi^{(\lambda 2)}$, the eigen-solutions belonging to the λ *rep*, $\boldsymbol{\Phi}^{(\lambda i)}=\boldsymbol{F}\boldsymbol{\Psi}^{(\lambda i)}$, are given by linear combinations of $\phi^{(\lambda 1)}$ and $\phi^{(\lambda 2)}$,

$$\boldsymbol{\Phi}^{(\lambda i)}=\phi^{(\lambda 1)}\cos\{\gamma_i(\lambda)\}+\phi^{(\lambda 2)}\sin\{\gamma_i(\lambda)\},\qquad i=1,\ 2. \tag{39}$$

By substituting $\boldsymbol{\Phi}^{(\lambda i)}$ into eq. (2), the eigenvalues $x_i(\lambda)$ and $\tan\{\gamma_i(\lambda)\}$ can be obtained as

$$\begin{aligned}
&x_{1,2}(A_1)=\frac{1}{2}\{\mu_+\pm m\sqrt{1+\xi_+^2}\},\\
&\tan\{\gamma_{1,2}(A_1)\}=\xi_+\pm\sqrt{1+\xi_+^2},\\
&x_{1,2}(A_2)=\frac{1}{2}\{\mu_-\pm m\sqrt{1+\xi_-^2}\},\\
&\tan\{\gamma_{1,2}(A_2)\}=\mu_-\mp\sqrt{1+\eta_-^2},\\
&x_{1,2}(B_1)=\frac{1}{2}\{\nu_+\pm n\sqrt{1+\eta_+^2}\},\\
&\tan\{\gamma_{1,2}(B_1)\}=\eta_+\mp\sqrt{1+\eta_+^2},\\
&x_{1,2}(B_2)=\frac{1}{2}\{\nu_-\pm n\sqrt{1+\eta_-^2}\},\\
&\tan\{\gamma_{1,2}(B_2)\}=\eta_-\pm\sqrt{1+\eta_-^2},
\end{aligned} \tag{40}$$

where

$$\begin{aligned}
&m=2(a-c)\cos\theta\sin 2\alpha,\\
&n=2(a+c)\cos\theta\sin 2\alpha,\\
&\mu_\pm=-2b\cos^2\theta\pm\{a+c-(a-c)\cos 2\alpha\}\sin^2\theta,\\
&\nu_\pm=2b\cos^2\theta\pm\{-a+c+(a+c)\cos 2\alpha\}\sin^2\theta,\\
&\xi_\pm=\{(a-c)\cos 2\alpha(1+\cos^2\theta)+(a+c)\sin^2\theta\pm 2b\sin^2\theta\}/m,\\
&\eta_\pm=\{(a+c)\cos 2\alpha(1+\cos^2\theta)+(a-c)\sin^2\theta\pm 2b\sin^2\theta\}/n.
\end{aligned} \tag{41}$$

since $\Psi_{0\sigma}^{(\lambda i)}$ and $\Psi_{0\pi}^{(\lambda i)}$ are $\frac{1}{2}\cos\{\gamma_i(\lambda)\}$ and $\frac{1}{2}\sin\{\gamma_i(\lambda)\}$, respectively, we have

$$c_i(\lambda)=\frac{1}{2}\cos\{\gamma-\gamma_i(\lambda)\}, \tag{42}$$

where $c_i(\lambda)$ is the coefficient in eq. (37).

Acknowledgements

The author is greatly indebted to Mr. M. Kogiso and Prof. Y. Kainuma of Nagoya University for discussions of this subject.

References

1) M. Kogiso and H. Takahashi: J. Phys. Soc. Japan **42** (1977) 223.
2) R. W. James: *The Optical Principles of the Diffraction of X-rays,* (Bell and Sons, London, 1967).
3) N. Kato: Acta cryst. **11** (1958) 885.
4) E. J. Saccocio and A. Zajac: Phys. Rev. **139** (1965) A255.
5) E. J. Saccocio and A. Zajac: Acta cryst. **18** (1965) 478.
6) T. Joko and A. Fukuhara: J. Phys. Soc. Japan **22** (1967) 595.
7) C. J. Bradley and A. P. Cracknell: *The Mathematical Theory of Symmetry in Solids* (Clarendon Press, Oxford, 1972).
8) B. Post, S. L. Chang and T. C. Huang: Acta cryst. **A33** (1977) 90.

(Received october 12, 1978)