A Theoretical Approach to Dynamical Diffraction of X-rays in the Bragg Case with the Green’s Function Method

Hidenobu ISHIDA*1

*1 Department of Management and Information Sciences

The dynamical diffraction theory of X-rays for a distorted crystal with the Green’s function method is applied to the Bragg case. The transmitted and diffracted crystal waves are represented as the solutions of the integral equations using the Green’s function. For a perfect crystal, the most exact form of the solution of the equations is given by the Green’s function and its derivatives, and the waves are analytically expressed by using them. The results can be applied in a general case where the amplitude modulation of the incident wave is not negligibly small compared with the wave vector. If the amplitude modulation is small, those results are reduced essentially to the same as those given by Takagi’s theory.

Key Words: X-rays, Dynamical Diffraction, Bragg Case, Maxwell’s Equation, Green’s Function

1. Introduction

Recently, the dynamical diffraction theory of X-rays for a largely distorted crystal was given by the present author(1)(2). In the theory, the crystal waves are expressed by a sum of modulated waves with amplitude modulation, the amplitudes of which vary slowly. The validity limit for the slowly varying assumption is the order of the size of several times of atomic layers, where the amplitude functions are considered to be almost constant. Before this theory, the idea of modulated waves for dynamical theory was used in the expansion of the Maxwell’s equation developed by Takagi(3). But the validity limit of Takagi’s theory is at most in the order of sub-micron, much restrictive compared with this theory. The fundamental equations are deduced from Maxwell’s equation for the electric field by using modulated waves. To obtain the solution of the fundamental equations, the Green’s function method is introduced. The crystal waves are related to the Green’s function by integral equations based on the Green’s formula of vector type. It was shown that in the Laue case the integral equations may give the solution of the waves by the forward propagating Green’s function (2), and that the crystal waves for a perfect crystal are analytically obtained using the Green’s function (4). In the present paper, the dynamical theory using the Green’s function is applied to the Bragg case. The boundary conditions for the Bragg case are different from those for the Laue case. The procedure to get the wave becomes rather complex compared with the Laue case, as shown in detail in the present paper.

2. Fundamental Equations in Two Wave Approximation

The fundamental equations (1) which describe the behavior of dynamical diffraction of X-rays in a perfect or distorted crystal are given in the two wave approximation using the "transverse wave approximation", (1)(4) by

\[
\begin{align*}
\nabla^2 E_0^{(t)}(r) + k^2 E_0(r) + k^2 \chi_0 E_0^{(t)}(r) + k^2 \chi\cdot (r-u(r))(E_0^{(t)}(r) = 0 \), \\
\nabla^2 E_h^{(t)}(r) + k^2 E_h(r) + k^2 \chi_0 E_h^{(t)}(r) + k^2 \chi\cdot (r-u(r))(E_h^{(t)}(r) = 0 \)
\end{align*}
\]

(1)

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*1 経済情報学科
E-mail: isidah@fukui-ut.ac.jp
where \( r \) is any point in the crystal, \( k \) is \( 2\pi \) times the wave number of the X-rays, \( \mathbf{h} \) is the reciprocal lattice vector, \( \chi_0 \), \( \chi_h \), and \( \chi_{-h} \) are the Fourier coefficients of crystal polarizability, \( \mathbf{E}_0 \) and \( \mathbf{E}_h \) are the electric field vectors representing the transmitted and diffracted components of a crystal wave given by

\[
E(r) = E_0(r) + E_h(r) .
\]  

(2)

\( E_0(r) \) and \( E_h(r) \) are their transverse wave components and \( \mathbf{u} \) is the displacement vector of the crystal lattice. Each of the transmitted and diffracted crystal waves is expressed with modulation amplitude and constant carrier wave vector as

\[
E_0(r) = \varphi_0(r) \exp(i\mathbf{k}_0 \cdot \mathbf{r}) , \quad E_h(r) = \varphi_h(r) \exp(i\mathbf{k}_h \cdot \mathbf{r}) ,
\]  

(3)

where \( \varphi_0(r) \) and \( \varphi_h(r) \) are the amplitude vector functions of two crystal waves, and \( \mathbf{k}_0 \) and \( \mathbf{k}_h \) are the constant wave vectors, \( \mathbf{k}_0 \) being related to \( \mathbf{k}_h \) by

\[
\mathbf{k}_h = \mathbf{k}_0 + \mathbf{h} .
\]  

(4)

\( E_0 \) and \( E_h \) are expanded to

\[
E_g(r) = \int_{V_0^+} E_g(\kappa) \exp(i\mathbf{k}_g \cdot \mathbf{r}) \frac{d\kappa}{(2\pi)^3} ,
\]  

(5)

where \( g = 0, h \) and \( V_0^+ \) is the space of the unit cell for the reciprocal lattice of a crystal, \( K_g \) being

\[
K_g = \mathbf{k}_g + \mathbf{\kappa} .
\]  

(6)

With respect to the polarizability, the reciprocal lattice component of \( \chi(r) \), that is, \( \chi_g \exp(-i\mathbf{g} \cdot \mathbf{u}(r)) \) is expanded to

\[
\chi_g \exp(-i\mathbf{g} \cdot \mathbf{u}(r)) = \int \chi_g(\kappa) \exp(i\kappa \cdot \mathbf{r}) \frac{d\kappa}{(2\pi)^3} .
\]  

(7)

The amplitude functions \( \varphi_0(r) \) and \( \varphi_h(r) \) are assumed to change slowly. It is also assumed for the displacement \( \mathbf{u}(r) \) to be slowly varying in the same meaning. The validity of this assumption is shown quantitatively as

\[
E_g(\kappa) = 0 , \quad \chi_g(\kappa) = 0 , \quad |\kappa| > \kappa_0 ,
\]  

(8)

where \( \kappa_0 = 2\pi/(3a_{\text{max}}) \), \( a_{\text{max}} \) being the longest side length of the three sides constituting a unit cell of the crystal. In typical case, \( a_{\text{max}} \approx 0.2 \) \( \text{nm} \) and then the lower limit of the macroscopic range becomes \( 2\pi/\kappa_0 \approx 3 a_{\text{max}} \approx 1 \) \( \text{nm} \). This value is much smaller than the application limit of the previous theory\(^3\).

When the Fourier component vector \( \mathbf{E}_g(\kappa) \) is expressed as a sum of the components of three independent polarizations, it may be shown as

\[
E_g(\kappa) = E_{1g}(\kappa)|e^1_g(\kappa)| + E_{2g}(\kappa)|e^2_g(\kappa)| + E_{3g}(\kappa)|e^3_g(\kappa)| ,
\]  

(9)

where \( |e^1_g(\kappa)| \) and \( |e^2_g(\kappa)| \) are two independent polarization vectors perpendicular to \( K_g \), i.e., polarization vectors for the transverse components of \( \mathbf{E}_g(\kappa) \), and \( |e^3_g(\kappa)| \) is the longitudinal polarization vector parallel to \( K_g \). Substitution of eq. (5) into eq. (1) using eq. (9) gives for the transverse components

\[
\left\{ k^2(1 + \chi_0) - K_g^2 \right\} E_0^\mu(\kappa) + k^2 \sum_{\nu = 1,2} \frac{C_{\nu0}^{\mu\nu}(\kappa,\kappa')\chi_{-h}(\kappa') E_h^\nu(\kappa - \kappa')}{(2\pi)^3} = 0 ,
\]  

\[
\left\{ k^2(1 + \chi_0) - K_g^2 \right\} E_h^\mu(\kappa) + k^2 \sum_{\nu = 1,2} \frac{C_{\nu0}^{\mu\nu}(\kappa,\kappa')\chi_h(\kappa') E_0^\nu(\kappa - \kappa')}{(2\pi)^3} = 0 ,
\]  

(10)

where \( \mu = 1, 2 \), and \( C_{\nu0}^{\mu\nu}(\kappa,\kappa') = \langle e^\nu_g(\kappa)|e^\nu_g(\kappa-\kappa') \rangle \).

Equations (10) are the fundamental equations for the Fourier coefficients of the two crystal waves.
3. Integral equation for wave filed using the Green’s Function

Corresponding to the fundamental equations in the two wave approximation (1), the fundamental equations of the Green’s function \(^{(1)}\) are given using the “transverse wave approximation”\(^{(1, 2)}\) by

\[
\nabla^2 G^{(1)}_{gg'}(r, r') + k^2 G_{gg'}(r, r') + k^2 \sum_{\mathbf{g} = 0, h} \chi_{gg'} \exp \{i (\mathbf{g} - \mathbf{g'}) \cdot (r - u(r)) \} G^{(1)}_{gg'}(r, r') = - \Delta_{gg'}(r, r') ,
\]

(11)

where \( \mathbf{g}, \mathbf{g}' = 0, h \) and \( \Delta_{gg'}(r, r') \) is defined by

\[
\Delta_{gg'}(r, r') = \sum_{\mu, \nu = 1}^{3} \iint \delta_{\mu\nu} \delta_{gg'} \delta(\mathbf{k} - \mathbf{k}') \exp \{i K_{g} \cdot r - i K'_{g'} \cdot r'\} |e_{\mu}^{g}(\mathbf{k})| |e_{\nu}^{g'}(\mathbf{k}')| d\mathbf{k} \frac{d\mathbf{k}'}{(2\pi)^3} ,
\]

(12)

with \( K_{g} = k_{g} + \mathbf{k} \) and \( K'_{g'} = k_{g'} + \mathbf{k}' \). \( G_{gg'} \) is the \((\mathbf{g}, \mathbf{g}')\)-th component wave of the Green’s function given by

\[
G(r, r') = \sum_{\mathbf{g}, \mathbf{g}' = 0, h} G_{gg'}(r, r') , \quad G_{gg'}(r, r') = \psi_{gg'}(r, r') \exp \{i k_{g} \cdot r - i k_{g'} \cdot r'\} .
\]

(13)

\( G^{(1)} \) means the transverse component of \( G \), and \( \psi_{gg'} \) is the modulation amplitude assumed to be slowly varying for each variable. The Green’s function is related to the crystal wave by

\[
E_{g}(r) = \sum_{\mathbf{g} = 0, h} \iint \left( G_{gg'}^{(1)}(r, r') \frac{\partial E_{g'}^{(e)}(r')}{\partial \mathbf{n}'} - \frac{\partial G_{gg'}^{(1)}(r, r')}{\partial \mathbf{n}'} E_{g'}^{(e)}(r') \right) dS' ,
\]

(14)

where \( g = 0, h \) and \( G^{(1)} \) is a function called “forward propagation Green’s function”, which consists of only the transverse waves propagating to front.\(^{(2)}\)

If the Green’s function is expanded to a Fourier series

\[
G_{gg'}(r, r') = \sum_{\mu, \nu = 1}^{3} \iint G_{gg'}^{(1)}(\mathbf{k}, \mathbf{k}') \exp \{i K_{g} \cdot r - i K'_{g'} \cdot r'\} \frac{d\mathbf{k}}{(2\pi)^3} \frac{d\mathbf{k}'}{(2\pi)^3} ,
\]

(15)

then \( G^{(1)} \) is given as a sum of the transverse components propagating to front by

\[
G_{gg'}^{(1)}(r, r') = \sum_{\mu, \nu = 1}^{3} \iint G_{gg'}^{(1)}(\mathbf{k}, \mathbf{k}') \exp \{i K_{g} \cdot r - i K'_{g'} \cdot r'\} \frac{d\mathbf{k}}{(2\pi)^3} \frac{d\mathbf{k}'}{(2\pi)^3} ,
\]

(16)

where \( \eta_{gg'} > 0 \) means

\[
\eta_{gg'}(\mathbf{k}, \mathbf{k}') \equiv (K_{g} + K'_{g'}) \cdot (r - r') > 0 .
\]

(17)

\( S \) is the surface of a crystal, and \( \mathbf{n}' \) is the unit vector normal to the crystal surface toward the outer direction. \( E_{g}^{(e)}(\mathbf{g} = 0, h) \), that is, \( E_{g}^{(e)} \) and \( E_{h}^{(e)} \) are the incident wave and the diffracted wave in vacuum given by

\[
E_{g}^{(e)}(r) = \Phi_{g}^{(e)}(r) \exp \{i K_{g} \cdot r\} , \quad E_{h}^{(e)}(r) = \Phi_{h}^{(e)}(r) \exp \{i K_{h} \cdot r\} ,
\]

(18)

respectively, with the amplitudes of varying slowly. By the boundary condition of the wave function, if the incident wave is assumed to incident with not a small angle to the crystal surface, the amplitude and its normal derivative of the wave function may be assumed to be continuous on the crystal surface \( S \) as follows:

\[
E_{g} = E_{g}^{(e)} , \quad \frac{\partial}{\partial n} E_{g} = \frac{\partial}{\partial n} E_{g}^{(e)} , \quad g = 0, h .
\]

(19)

In two-wave approximation for the Laue case, for a both sides crystal made from the entrance surface and the back surface, the integral over the back surface in eq. (14) is neglected so that the integral only over the entrance surface is significant. In addition, the diffracted wave on the entrance surface does not exit and is emitted from the back surface, and therefore, if the entrance surface is referred as \( \Gamma_{1} \), equation (14) becomes\(^{(2, 4)}\)
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\[ E_g(r) = \int \left\{ G_g^{(0)}(r, r') \frac{\partial E^{(0)}(r')}{\partial n'} - \frac{\partial G_g^{(0)}(r, r')}{\partial n'} E^{(e)}(r') \right\} dS', \quad g = 0, h. \]  

(20)

This gives the solution of the fundamental equation (1).

On the other hand, in the Bragg case the situation is very different from that in the Laue case, since the diffracted wave does not vanish on the entrance surface and the integral part of eq. (14) over the back surface is not negligible. Even if the crystal is enough thick to neglect the back surface integral, the diffracted wave still remains as unknown wave function. In other words, in this case equation (14) is rewritten, replacing the vacuum diffracted wave to the crystal wave, as

\[ E_g(r) = \int \left\{ G_g^{(0)} \frac{\partial E^{(e)}(r')}{\partial n'} - \frac{\partial G_g^{(0)}(r, r')}{\partial n'} E^{(e)}(r') \right\} dS' + \int \left\{ G_{gh}^{(0)} \frac{\partial E^{(e)}(r')}{\partial n'} - \frac{\partial G_{gh}^{(0)}(r, r')}{\partial n'} E^{(e)}(r') \right\} dS', \quad g = 0, h. \]  

(21)

This is the integral equation to be solved to obtain the solution of the fundamental equation of the crystal wave. The process to get solution is a little troublesome, because at first the Green's function should be obtained in an explicit form and then the integral equation should be solved. The Fourier coefficients of the forward propagation Green's function is determined by

\[ \left\{ k^2 - K_g^{(2)} \right\} G_{gg'}^{(2)}(\kappa, \kappa') + k^2 \sum_{g'=h, \mu=1}^{2} \int C_{gg'}^{(2)}(\kappa, \kappa') \chi_{g'-\mu}(\kappa') G_{g'g}(\kappa, \kappa') \frac{d\kappa'}{(2\pi)^3} \]

\[ = -(2\pi)^3 \delta_{gg'} \delta_{\mu, \nu} \delta(\kappa - \kappa'), \quad \mu, \nu = 1, 2, \quad g, g' = 0, h. \]  

(22)

This equation is derived by substitution of eqs. (15) and (16) into eq. (11).

4. Green's Function in Perfect Crystal

In the case of a perfect crystal, i.e., the case where a crystal is undistorted so that the lattice displacement vector \( \mathbf{u}(r) \) equals to 0, \( \chi_g(\kappa) = (2\pi)^3 \chi_g \delta(\kappa) \). If the polarization vector \( e_\sigma(r) \) is chosen to be for \( \sigma \)-polarization and \( e_\pi(r) \) to be for \( \pi \)-polarization, then \( C_{10}^{(2)}(\kappa, 0) = C_{01}^{(2)}(\kappa, 0) = 1, C_{20}^{(2)}(\kappa, 0) = C_{02}^{(2)}(\kappa, 0) = e_\pi(\kappa) \cdot e_\pi(\kappa), \) and \( C_{00}^{(2)}(\kappa, 0) = C_{20}^{(2)}(\kappa, 0) = 0 \) so that equation (10) reduces to the well-known determination equation for crystal waves \( \delta(\kappa - \kappa') \)

\[ \left\{ k^2(1 + \chi_0) - K_g^{(2)} \right\} E_0^{(e)}(\kappa) + k^2 C_\mu \chi_{-h} E_h^{(e)}(\kappa) = 0, \quad \mu = 1, 2, \]  

(23)

\[ \left\{ k^2(1 + \chi_0) - K_h^{(2)} \right\} E_h^{(e)}(\kappa) + k^2 C_\mu \chi_{h} E_0^{(e)}(\kappa) = 0, \]  

where \( C_\mu \) is the polarization factor given by \( C_1 = 1 \) for \( \sigma \)-polarization and \( C_2 = e_\pi(\kappa) \cdot e_\pi(\kappa) = \cos 2\theta_h(\kappa) \) for \( \pi \)-polarization, with \( 2\theta_h(\kappa) \) being the angle between the directions of \( K_0 \) and \( K_h \). Similarly, equations (22) gives

\[ \left\{ k^2(1 + \chi_0) - K_g^{(2)} \right\} G_{g0}^{(2)}(\kappa, \kappa') + k^2 C_\mu \chi_{-h} G_{h0}^{(2)}(\kappa, \kappa') = -(2\pi)^3 \delta_{\mu, \nu} \delta(\kappa - \kappa'), \quad \mu, \nu = 1, 2, \]  

(24)

\[ \left\{ k^2(1 + \chi_0) - K_h^{(2)} \right\} G_{h0}^{(2)}(\kappa, \kappa') + k^2 C_\mu \chi_h G_{g0}^{(2)}(\kappa, \kappa') = 0, \]  

and

\[ \left\{ k^2(1 + \chi_0) - K_g^{(2)} \right\} G_{g0}^{(2)}(\kappa, \kappa') + k^2 C_\mu \chi_{-h} G_{h0}^{(2)}(\kappa, \kappa') = 0, \quad \mu, \nu = 1, 2, \]  

(25)

Since equations (24) and (25) are sets of linear equations with unknown \( G_{gg'}^{(2)} \)'s, the solutions may be given by

\[ G_{gg'}^{(2)}(\kappa, \kappa') = (2\pi)^3 \delta_{\mu, \nu} \delta(\kappa - \kappa') G_{gg'}^{(e)}(\kappa), \quad g, g' = 0, h. \]  

(26)

Here, if \( K = K_0 + \kappa = K_0 \) is used,
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\[ G_{00}^{\mu}(\kappa) = -\left\{ k^2 (1 + \chi_0) - K_h^2 \right\} / D(\mathbf{K}) \equiv G_{00}^{\mu}(\mathbf{K}), \] (27)

\[ G_{h0}^{\mu}(\kappa) = k^2 C_\mu \chi_h / D(\mathbf{K}) \equiv G_{h0}^{\mu}(\mathbf{K}), \] (28)

\[ G_{oh}^{\mu}(\kappa) = k^2 C_\mu \chi_h / D(\mathbf{K}) \equiv G_{oh}^{\mu}(\mathbf{K}), \] (29)

\[ G_{hh}^{\mu}(\kappa) = -\left\{ k^2 (1 + \chi_0) - K^2 \right\} / D(\mathbf{K}) \equiv G_{hh}^{\mu}(\mathbf{K}), \] (30)

with \( D(\mathbf{K}) \) being

\[ D(\mathbf{K}) = \{ k^2 (1 + \chi_0) - K^2 \} - k^4 C_\mu^2 \chi_h \chi_{-h}. \] (31)

By using eqs. (27) - (31), substituting eq. (26) into eq. (16) and performing the integration, \( G_{00}, G_{h0}, G_{oh}, \) and \( G_{hh} \) can be obtained analytically. Here, an approximation is introduced to extend the integral range of eq. (16) from the unit cell volume in the reciprocal lattice space to infinite space. Influence of such approximation on the integral equation (21) is negligible, because the integral region is restricted naturally by the assumption of slowly varying for the crystal waves to the range given by (8). Furthermore, as seen from eqs. (27) - (31), \( G_{gpg}(\mathbf{k}, \mathbf{g} = 0, \mathbf{h}) \) are all the functions of \( \mathbf{K} = K_0 + \kappa \). Therefore, let the integration variables change from \( \kappa \) to \( \mathbf{K} \) and let \( G_{gpg}(\mathbf{K}) \) be used instead of \( G_{gpg}(\kappa) \). Then, equation (16) may be approximated by

\[ G^{\mu}_{gpg}(\mathbf{r}, \mathbf{r}') = \sum_{\mu=1}^{2} \int_{\eta_{gpg}(\mathbf{K}) > 0} G_{gpg}^{\mu}(\mathbf{K}) \psi_{gpg}^{\mu}(\mathbf{K}, \mathbf{r}, \mathbf{r}') \frac{d\mathbf{K}}{(2\pi)^3}, \quad \mathbf{g}, \mathbf{g}' = 0, \mathbf{h}, \] (32)

where

\[ \psi_{gpg}^{\mu}(\mathbf{K}, \mathbf{r}, \mathbf{r}') = \exp(i\mathbf{K} \cdot (\mathbf{r} - \mathbf{r}') + i \mathbf{g} \cdot \mathbf{r} - i \mathbf{g}' \cdot \mathbf{r}') |e_{g}^{\mu}(\mathbf{K})| |e_{g'}^{\mu}(\mathbf{K})|, \] (33)

and the integral is over the total space constrained by the condition \( \eta_{gpg}(\mathbf{K}) = \eta_{gpg}(\mathbf{K}, \mathbf{K}) = (2\mathbf{K} + \mathbf{g} + \mathbf{g}') \cdot (\mathbf{r} - \mathbf{r}') > 0 \). In equation (32), the integrations of \( G_{00} \) and \( G_{h0} \) are shown in another paper \(^4\) and the integration process of \( G_{oh} \) and \( G_{hh} \) may be similarly executable so that the results may be summarized as follows:

\[ G^{\mu}_{gpg}(\mathbf{r}, \mathbf{r}') = \delta_{gpg}G_{00}(\mathbf{r} - \mathbf{r}') \eta_{gpg}(\phi, \phi) + \sum_{\mu=1}^{2} k \cos \theta_B \int_{\eta_{gpg}(\phi) > 0} \frac{d\phi}{2\pi} W_{gpg}^{\mu}(s_0(\phi), s_h(\phi)) \psi_{gpg}^{\mu}(\mathbf{K}, \mathbf{r}, \mathbf{r}'), \] (34)

where \( \eta_{gpg}(\phi) \equiv \eta_{gpg}(\kappa(\phi)) = (2\mathbf{K} + \mathbf{g} + \mathbf{g}') \cdot (\mathbf{r} - \mathbf{r}') \) and, if \( s_0 > 0 \) and \( s_h > 0 \),

\[ W_{00}^{\mu}(s_0, s_h) = -i C(X_h X_0)^{1/2} e^{ikx_0(s_0 + s_h)/2} \sqrt{S_0 S_h} \int_{J} (\beta \sqrt{S_0 S_h}), \] (35)

\[ W_{h0}^{\mu}(s_0, s_h) = -i C X_h e^{ikx_0(s_0 + s_h)/2} \int_{J} (\beta \sqrt{S_0 S_h}), \] (36)

\[ W_{oh}^{\mu}(s_0, s_h) = -i C X_0 e^{ikx_0(s_0 + s_h)/2} \int_{J} (\beta \sqrt{S_0 S_h}), \] (37)

\[ W_{hh}^{\mu}(s_0, s_h) = -i C(X_h X_0)^{1/2} e^{ikx_0(s_0 + s_h)/2} \sqrt{S_0 S_h} \int_{J} (\beta \sqrt{S_0 S_h}). \] (38)
If \( s_0 < 0 \) or \( s_h < 0 \), \( W^{\mu}_{\eta\Theta\varphi}(s_0, s_h) = 0 \). Here, \( J_0 \) and \( J_1 \) are the Bessel functions of the 0-th and 1-st order, respectively, and \( \beta = kC(\chi_h \chi) \). \( \Lambda^{(3)} \) is the \( 3 \times 3 \) unit matrix tensor and \( G_0(r - r') \) is a spherical wave function given by

\[
G_0(r - r') = \frac{e^{ik(1 + X_0)(r - r')}}{4\pi |r - r'|}.
\]

(39)

\( \theta_B \) is the Bragg angle given by \( 2d \sin \theta_B = \lambda \), and \( C \) is the polarization factor given by \( C = 1, \cos 2\theta_B (\mu = 1, 2) \). As shown in Fig. 1, when we use an orthogonal coordinate system \( (\xi, \eta, \zeta) \) where \( \xi \)-axis is taken along the reciprocal lattice vector \( h \) and \( \xi - \zeta \) plane is a plane made by \( k_0 \) and \( k_h \), the coordinates of points \( r \) and \( r' \) are expressed as \( r = (\xi, \eta, \zeta) \) and \( r' = (\xi', \eta', \zeta') \). The variables \( s_0(\phi) \) and \( s_h(\phi) \) of \( W^{(\mu)}_{\eta\Theta\varphi} \) in eq. (34) are defined by

\[
s_0(\phi) = \frac{1}{2 \cos \theta_B} \left( \frac{1}{\xi - \zeta} \cos \phi + (\eta - \eta') \sin \phi \right),
\]

\[
s_h(\phi) = \frac{1}{2 \cos \theta_B} \left( \frac{1}{\xi - \zeta} \cos \phi + (\eta - \eta') \sin \phi \right).
\]

(40)

The wave vector \( k(\phi) \) is given in the \( \xi\eta\zeta \) coordinate system by

\[
k(\phi) = (k \cos \theta_B \cos \phi, k \cos \theta_B \sin \phi, -k \sin \theta_B).
\]

(41)

Thus, the Green’s functions have been expressed analytically. The analytical expressions presented here have still integral forms, which integrations will be executed with the saddle point method in good approximation in later section. However, for convenience to get the solution of the integral equation (21), it is better to hold the exact form as possible for a while.

5. Solution in Perfect Crystal

When the Fourier coefficients of \( G_{00}, G_{h0}, G_{0h} \) and \( G_{hh} \) are given by eqs. (27) - (30), then the solution of the integral equations (21) for a flat crystal may be given as shown in Appendix A by

\[
E_g(r) = 2 \int \left\{ \frac{\partial G^{(c)}_{\eta\Theta\varphi}(r, r')}{\partial z'} - \frac{1}{k^2 \chi - h} (\nabla_{z'} + k^2 (1 + X_0)) \left( \frac{\partial G_{gh}(r, r')}{\partial z'} - e^{i k r'} \right) \right\} E_0^{(c)}(r') dS',
\]

(42)

where \( g = 0, h \) and, \( G^{(c)}_{gh} \) is defined using the Fourier component of \( G_{gh} \) by

\[
G^{(c)}_{gh}(r, r') = \sum_{\mu=1}^{2} \int_{C} \frac{1}{C} G^\mu_{gh}(\kappa) \Psi^\mu_{gh}(K, r, r') \frac{dk}{(2\pi)^3},
\]

(43)

with

\[
\Psi^\mu_{gh}(K, r, r') = \exp[iK \cdot (r - r') + i g \cdot r - i h \cdot r']|e^\mu_g(K)| \left\{ e^\mu_0(K) \right\}, \quad K = k_0 + k.
\]

(44)

\( z' \) is the axis normal to the crystal surface to the inward direction.

The integration of eq. (43) is analogous to that of eq. (32) for \( G_{0h} \) and \( G_{hh} \). The result is shown by

\[
G^\mu_{0h}(r, r') = \sum_{\mu=1}^{2} \frac{k \cos \theta_B}{C} \frac{d\phi}{\eta_{0h}(\phi) > 0} \frac{d\phi}{2\pi} W^{\mu}_{0h}(s_0(\phi), s_h(\phi)) \Psi^\mu_{0h}(k(\phi), r, r'),
\]

(45)

and

\[
G^\mu_{hh}(r, r') = \sum_{\mu=1}^{2} \frac{k \cos \theta_B}{C} \frac{d\phi}{\eta_{hh}(\phi) > 0} \frac{d\phi}{2\pi} \left\{ \frac{e^{i\theta_0(\phi)/2}}{2\sin 2\theta_B} \delta(s_0(\phi)) + W^{\mu}_{hh}(s_0(\phi), s_h(\phi)) \right\} \Psi^\mu_{hh}(k(\phi), r, r').
\]

(46)

Substitution of eq. (45) into the second integral terms of eq. (42) gives for \( g = 0 \)
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\[
- \frac{1}{k^2 X_h} \left( \nabla^2 + k^2 \right) \left( \frac{\partial G_{\text{oh}}(r,r')}{\partial z'} e^{ikr} \right) = \sum_{\mu=1}^{2} \frac{k \cos \theta_B}{C} \int_{\eta_{\text{oh}}(\phi)>0} \frac{d\phi}{2\pi} i k_{\text{hh}}(\phi) W_{\text{gh}}(s_0(\phi), s_h(\phi)) \left\{ 2ik(\phi) \cdot \nabla_r W_{\text{oh}}^{(\mu)} - k^2 X_0 W_{\text{oh}}^{(\mu)} \right\},
\]

where \( k_{\text{hh}}(\phi) = k_0(\phi) + h_3 \) and the second derivative term \( \nabla^2 W_{\text{oh}}'^{\mu} \) is neglected because it is negligibly small compared with the other terms. Similarly, this approximation may be applied to the case of \( g = h \). After all, using the analytical forms of \( W_{\text{oh}}^{(\mu)} \) and \( W_{\text{gh}}^{(\mu)} \) given by eqs. (37) and (38), we get the following equations from eq. (42):

\[
E_0(r) = 2 \int_{\Gamma_1} \frac{\partial G_{00}^{(\mu)}(r,r')}{\partial z'} E_0^{(e)}(r')dS', \quad E_h(r) = 2 \int_{\Gamma_1} \frac{\partial G_{0h}^{(\mu)}(r,r')}{\partial z'} E_0^{(e)}(r')dS',
\]

where

\[
E_{00}^{(\mu)}(r,r') = G_0(r-r')I^{(3)} + \sum_{\mu=1}^{2} \int_{\eta_{00}(\phi)>0} W_{00}(s_0(\phi), s_0(\phi)) \int_{\eta_{00}(\phi)>0} W_{0h}(s_0(\phi), s_h(\phi)) \left\{ e^{ik(\phi)}(r-r') \right\} \left\{ e^{ik(\phi)}(r-r') \right\} \frac{d\phi}{2\pi},
\]

and

\[
E_{0h}^{(\mu)}(r,r') = \sum_{\mu=1}^{2} \int_{\eta_{0h}(\phi)>0} W_{0h}(s_0(\phi), s_h(\phi)) \int_{\eta_{0h}(\phi)>0} W_{0h}(s_0(\phi), s_h(\phi)) \left\{ e^{ik(\phi)}(r-r') \right\} \left\{ e^{ik(\phi)}(r-r') \right\} \frac{d\phi}{2\pi},
\]

with

\[
W_{0h}(s_0(\phi), s_h(\phi)) = \left\{ 2ik(\phi) \cdot \nabla_r W_{0h}^{(\mu)} - k^2 X_0 W_{0h}^{(\mu)} \right\} / k^2 C X_h .
\]

\( \gamma_0(\phi) = k_0(\phi)/k \) and \( \gamma_h(\phi) = -k_{\text{hh}}(\phi)/k = -(k_0(\phi) + h_3)/k \), namely, using the relation of the coordinate systems of \((x,y,z)\) and \((\xi, \eta, \zeta)\), \( \xi = x \cos \alpha - z \sin \alpha \), \( \eta = -y \) and \( \zeta = -x \sin \alpha - z \cos \alpha \) as shown in Fig. 2,

\[
\gamma_0(\phi) = \sin \theta_B \cos \zeta - \cos \theta_B \cos \phi \sin \alpha, \quad \gamma_h(\phi) = \sin \theta_B \cos \alpha + \cos \theta_B \cos \phi \sin \alpha,
\]

\( \alpha \) being the angle between \( \xi - \eta \) and \( x - y \) planes, that is, the net plane of the crystal lattice and the crystal surface, with \( -\theta_B < \alpha < \theta_B \). In the Bragg case, it should be always that \( \gamma_h(\phi) > 0 \) because the diffracted wave is diffracted from the entrance surface and so \( k_{\text{hh}}(\phi) < 0 \), which limits the integral ranges of the second integral terms eqs. (48) and (49).

Here, let us integrate eqs. (48) and (49) with the saddle point method, approximately. In this case, there exist two saddle points \( \phi = \phi_0 \) and \( \phi = \phi_0 + \pi \), as seen that \( k(\phi) \cdot (r-r') = k \cos \theta_B \cdot r(\phi, \phi') \cdot \cos(\phi - \phi_0) - k \sin \theta_B \cdot (\zeta - \zeta'), \) with \( \tan \theta_B = (\eta - \eta') / (\xi - \xi') \). The latter saddle point may be excluded, if we select the saddle point which gives the wave vector closer to the wave vector \( k_0 = k(\phi = 0) \) of the incident wave vector, when \( (\eta - \eta') \approx 0 \), i.e., \( \phi_0 \equiv 0 \). Thus the saddle point integrations of eqs. (48) and (49) give

\[
E_{00}^{(\mu)}(r,r') = \frac{e^{ik(1+X_0)^{1/2}r-r'}}{4\pi|r-r'|} I^{(3)} + \sum_{\mu=1}^{2} e^{-\frac{\pi}{4}} \sqrt{\frac{k \cos \theta_B}{2\pi \rho(r-r')}} W_{00}^{(\mu)}(s_0(\phi), s_h(\phi)) \left\{ e^{ik(\phi)}(r-r') \right\} \left\{ e^{ik(\phi)}(r-r') \right\} \times \exp\left\{ ik \cos \theta_B \cdot r(\phi, \phi') - i k \sin \theta_B \cdot (\zeta - \zeta') \right\} e^{ik(\phi)}(r-r') \left\{ e^{ik(\phi)}(r-r') \right\} ,
\]

\( \therefore 173 \)
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and

\[ G^{(B)}_{h0}(r, r') = \sum_{\mu=1}^{2} e^{-i\frac{\pi}{4}} \frac{k \cos \theta_B}{2\pi r (r - r')} W^{(B)\mu}_{h0}(s_0(r - r'), s_h(r - r')) \exp(ik \cos \theta_B \cdot \rho(r - r')) \]

\[ - i k \sin \theta_B \left( \xi - \xi' \right) + i \frac{h}{\rho} \left| e_{h0}(\mathbf{k}(\phi_0)) \right| \left( e_{h0}(\mathbf{k}(\phi_0)) \right) , \]

where \( W^{(B)\mu}_{h0}(s_0, s_h) = W^{(B)\mu}_{0h}(s_0, s_h) - \gamma_h y_0 \gamma_0 \gamma_h^{(B)\mu}(s_0, s_h), \quad (g = 0, h) \). When \( s_0 > 0 \) and \( s_h > 0 \), \( W^{(B)\mu}_{h0} \) are explicitly rewritten using eqs. (35)-(38) and (50) as

\[ W^{(B)\mu}_{00}(s_0, s_h) = \frac{\gamma_h}{\gamma_0 2k \sin 2\theta_B} \delta(s_0) - i \frac{C \chi_h \chi_{-h}}{4 \sin 2\theta_B} \frac{1}{2} e^{-i \frac{kx_0(s_0 + s_h)}{2}} \left\{ \frac{s_0}{s_h} - \frac{\gamma_h}{\gamma_0} \right\} \frac{s_h}{s_0} J_1 \left( \beta \sqrt{s_0 s_h} \right) , \]

and

\[ W^{(B)\mu}_{h0}(s_0, s_h) = \frac{\gamma_h}{\gamma_0 2k} C \chi_{-h} \sin 2\theta_B \delta(s_0) \]

\[ - \frac{C \chi_h}{4 \sin 2\theta_B} e^{-i \frac{kx_0(s_0 + s_h)}{2}} \left\{ \left( 1 - \frac{\gamma_h s_h}{\gamma_0 s_0} \right) J_1 \left( \beta \sqrt{s_0 s_h} \right) + 2 \frac{\gamma_h s_h}{\gamma_0 s_0} J_1 \left( \beta \sqrt{s_0 s_h} \right) \right\} . \]

If \( s_0 < 0 \) or \( s_h < 0 \), \( W^{(B)\mu}_{g0}(s_0, s_h) = 0 \). The factor \( \rho(r - r') \) in eqs. (52) and (53) is given by

\[ \rho(r - r') = \sqrt{(\xi - \xi')^2 + (\eta - \eta')^2} . \]

\[ s_0(r - r') \] and \( s_h(r - r') \) are given by

\[ s_0(r - r') = \frac{\rho(r - r')}{2 \cos \theta_B} - \frac{\xi - \xi'}{2 \sin \theta_B} , \quad s_h(r - r') = \frac{\rho(r - r')}{2 \cos \theta_B} + \frac{\xi - \xi'}{2 \sin \theta_B} . \]

Also, the wave vector \( \mathbf{k}(\phi_0) \) is defined using \( \tan \phi_0 = (\eta - \eta')/(\xi - \xi') \) as

\[ k(\phi) = (k \cos \theta_B \cos \phi_0, k \cos \theta_B \sin \phi_0, -k \sin \theta_B) . \]

The factor \( \gamma_h/\gamma_0 \) in eqs. (54) and (55) equals \( \gamma_h(\phi_0)/\gamma_0(\phi_0) \), when used in eqs. (52) and (53).

Thus, the crystal waves have been expressed analytically. In the Bragg case, it has been shown that the transmitted and diffracted waves may be expressed as eq. (47), using \( G^{(B)}_{00}(r, r') \) and \( G^{(B)}_{h0}(r, r') \), respectively. These results are applicable to the incident wave of arbitrary wave form within the validity of the assumption given by (8).

It should be noted that the delta functions appearing in eqs. (54) and (55) do not include any contributions to the integrals (47) so that they can be excluded from eqs. (54) and (55), because the half line \( s_0 = 0 \) \( (s_h > 0) \) exists out of the crystal in the Bragg case.

If the crystal waves are described with modulation amplitudes as in eq. (3), it is convenient to deduce expressions for the amplitudes of the crystal waves. In the present case, the wave vectors \( \mathbf{k}_0 \) and \( \mathbf{k}_h \) referred in eq. (3) are selected as

\[ \mathbf{k}_0 \equiv \mathbf{k}(\phi = 0) = (k \cos \theta_B, 0, -k \sin \theta_B) , \quad \mathbf{k}_h = \mathbf{k}_0 + \mathbf{h} = (k \cos \theta_B, 0, k \sin \theta_B) , \]

as shown in Fig.1. Then, the amplitude functions \( \psi^{(B)}_{00}(r, r') \) and \( \psi^{(B)}_{h0}(r, r') \) of \( G^{(B)}_{00} \) and \( G^{(B)}_{h0} \) may be deduced from eqs. (52) and (53) using

\[ \psi^{(B)}_{00}(r, r') = C^{(B)}_{00}(r, r') e^{-i k(\phi - \phi_0 - \xi') - i \theta} , \quad \psi^{(B)}_{h0}(r, r') = G^{(B)}_{h0}(r, r') e^{-i k\rho(r - r') - i \theta} . \]

Using the amplitude functions, the amplitudes of the two strong crystal waves may be expressed using eqs. (47) and (60) as
\[ \varphi_b(r) = 2 \int_{\Gamma_x} \left( \partial \varphi_{g0}(r,r')/\partial z' - i k r_0 \varphi_{g0}(r,r') \right) \Phi_0^{(e)}(r') dS', \quad g = 0, h, \quad (61) \]

where \( \Phi_0^{(e)} \) is the incident wave amplitude given by eq. (18). If the variation of \( \Phi_0^{(e)} \) is very small compared with \( k r_0 \),

\[ \varphi_b(r) = -2 i k \int_{\Gamma_x} r_0 \varphi_{g0}(r,r') \Phi_0^{(e)}(r') dS', \quad g = 0, h, \quad (62) \]

is derived from eq. (61), because the first integral term \( \partial \varphi_{g0}/\partial z' \cdot \Phi_0^{(e)} \) may be neglected.

6. Discussion

In the same manner as discussed in the Laue case\(^{(4)}\), we will discuss about the validity for the result given in the former section.

If the variation of the incident wave amplitude \( \Phi_0^{(e)} \) is negligible compared with the wave vector and the distribution of \( \Phi_0^{(e)} \) is homogeneous toward \( \eta \)-direction perpendicular to the incident plane made by \( k_0 \) and \( k_h \), then equation (62) is reduced to

\[ \varphi_b(\xi) = -2 i k \int_{\Gamma_x} r_0 \varphi_{g0}(\xi, x') \Phi_0^{(e)}(x') dx', \quad (63) \]

where \( \Phi_0^{(e)}(x) \) is the incident wave amplitude at any point \( x \) on the entrance surface in the incident plane, and \( \xi \) is any point in the crystal in the incident plane and \( \Gamma_x \) is the integral range for \( x \) (See Fig.2).

\( \varphi^{(b)} \) is given by the integral of \( \varphi^{(b)} \) integrated along \( \eta \), i.e.,

\[ \varphi_{g0}^{(b)}(\xi, \xi') = \int_{\Gamma_\eta} \varphi_{g0}^{(b)}(\xi, r') d\eta', \quad (64) \]

where \( \Gamma_\eta \) is the surface along \( \eta \). If \( \Gamma_\eta \) is infinitely extended, equation (64) may be integrated with the saddle point method, using the analytical forms of \( \varphi^{(b)} \) obtained by substituting eqs. (52) and (53) into eq. (60). The results become

\[ \varphi_{00}^{(b)}(\xi, \xi') = \frac{i \delta(s_h(\xi - \xi'))}{2k \sin 2 \theta_B} e^{i k s_{00}(\xi - \xi')/2} + \sum_{\mu=1}^{2} W_{00}^{(b)\mu}(s_0(\xi - \xi'), s_h(\xi - \xi')) [e^{\mu}_{0}(k_0)](e^{\mu}_{0}(k_0)), \quad (65) \]

\[ \varphi_{h0}^{(b)}(\xi, \xi') = \sum_{\mu=1}^{2} W_{h0}^{(b)\mu}(s_0(\xi - \xi'), s_h(\xi - \xi')) [e^{\mu}_{h}(k_0)](e^{\mu}_{h}(k_0)), \quad (66) \]

where

\[ s_0(\xi) = \frac{\xi}{2 \cos \theta_B} - \frac{\xi}{2 \sin \theta_B}, \quad s_h(\xi) = \frac{\xi}{2 \cos \theta_B} + \frac{\xi}{2 \sin \theta_B}. \quad (67) \]

The second term on the right-hand side of eq. (65) and the right-hand side of eq. (66) can be obtained by integrating with the saddle point method. The saddle point method is not used to get the first term on the right-hand side of eq. (65). Instead it is
obtained by approximately performing the Fourier integral of $G_0$, where the Fourier component $1/(K^2 - k^2(1 + \chi_0))$ is approximated by $1/(2K \cdot \delta K - k^2\chi_0)$ with $\delta K = K - k_0$.

According to eq. (63), when the incident wave is singly polarized and its amplitude width is very narrow, namely,

$$\varphi(x) = \delta(x) |e_{0}^\mu(k_0)|,$$

then the wave filed in a crystal is expressed as

$$\varphi(k) = -2i\epsilon_{r} G_{\varphi}^{(g)}(\xi, 0) |e_{0}^\mu(k_0)|, \quad g = 0, h.$$

Alternatively, using eqs. (54), (55), (65) and (66), it is expressed by the following equation:

$$\varphi_0(s_0, s_\hbar) = \left\{ \frac{\gamma_0}{\sin 2\theta_B} \delta(s_\hbar) - \frac{kC(\chi_0 \chi_\hbar)}{2 \sin 2\theta_B} \left( \frac{\gamma_0}{s_\hbar} - \gamma_\hbar \frac{s_\hbar}{s_0} \right) \right\} \left( \frac{\gamma_0}{s_\hbar - \gamma_\hbar} \frac{s_\hbar}{s_0} \right) \left( \beta \sqrt{s_0 s_\hbar} \right) e^{\frac{ikx_0(s_0 + s_\hbar)}{2}} |e_{0}^\mu(k_0)|,$$

$$\varphi_\hbar(s_0, s_\hbar) = \left\{ \frac{kC(\chi_0 \chi_\hbar)}{2 \sin 2\theta_B} \right\} \left( \frac{\gamma_0}{s_\hbar - \gamma_\hbar} \frac{s_\hbar}{s_0} \right) \left( \frac{\gamma_0}{s_\hbar - \gamma_\hbar} \frac{s_\hbar}{s_0} \right) \left( \beta \sqrt{s_0 s_\hbar} \right) e^{\frac{ikx_0(s_0 + s_\hbar)}{2}} |e_{0}^\mu(k_0)|,$$

where $s_0 = s_0(\xi), s_\hbar = s_\hbar(\xi)$ and $\gamma_0 = \gamma_0(0) = k_0/k$.

The result presented in this section is essentially the same as one shown by Takagi’s theory(7). Therefore, it may be concluded that the present dynamical theory using the Green’s function becomes an extension of Takagi’s theory.

7. Conclusion

In most of experimental studies of dynamical diffraction of X-ray the objects are to get some crystallographic or optical information by measuring only one diffracted wave of the two strong waves in the Laue case or in the Bragg case. In this sense, it is significant to show application of the Green’s function method to diffraction for the Bragg case.

In the Bragg case, a set of integral equations for the transmitted and diffracted waves in a crystal are deduced from the integral equations with the Green’s function. In the case of a perfect crystal, the analytical form of Green’s function is obtained, and using those and their derivatives the most exact form of the solution of the integral equations for the two waves is given. Substitution of the analytical form of the Green’s function and their derivatives into the integral form of the solution gives analytical expressions of the crystal waves. The results are applicable to a general case where the incident wave has any wave form within the validity of slowly varying in the scale of ~1 nm, and are different in this point from those given by Takagi’s theory, but are reducible to those.

Appendix

A. Derivation of eqs. (42)

Substitution of eq. (26) into eq. (16) gives

$$\mathbf{G}_{gg'}(r, r') = \sum_{\mu=1, \nu} \int \mathbf{G}_g^\mu(\mathbf{k}) e^{i\mathbf{k}(r-r') + ig_\mu \mathbf{s}(r-r')} |e_{g}^\mu(\mathbf{k})||e_{g'}^\mu(\mathbf{k})| d\mathbf{k},$$

(A1)

where $g_{gg'} = g_{gg'}(K, K)$. Here, the crystal is assumed to be a flat crystal, and let the z-axis be Along the direction normal to the entrance surface. In this integral, the integration about $\kappa_z$ can be performed easily with the residue integral method, if the zero points of the denominator $D(K)$ of $G_{gg'}^\mu(\mathbf{k})$ given by eqs. (27) - (30) are obtained.
These zero points are called dispersion points are shown as the intersection of the dispersion surfaces given by \( D(K) = 0 \) and the line \( K_i = K_i^* \), where \( K_i = k_{0i} + \kappa_i \) is the component of \( K \) parallel to the crystal surface, and \( K_i^* \) is a given vector such as the parallel component of the incident wave vector (See Fig. 3). The dispersion points exist near the dispersion sphere \( |K| = k(1 + X_0)^{1/2} \) or \( |K_i| = k(1 + X_0)^{1/2} \). Therefore, around these points, the polarization factor \( C_2 = \cos 2\theta_n(K) \) may be approximated by the \( C_2 \) for the \( \kappa \)-value at the cross point of \( K_i = k_{0i} + \kappa_i \) and the sphere, which is a function of \( K_i \) or \( \kappa_i \).

Then, the determination equation \( D(K) = 0 \) becomes a fourth-order equation with respect to \( \kappa_z \), and so the four \( \kappa_z \) roots exist as indicated by the dispersion points \( A_1, A_2, A_3 \) and \( A_4 \) in Fig. 3. In usual case where the incident wave incident on the crystal surface with not a small angle, two of them \( A_1 \) and \( A_4 \) far from the Laue point \( L \), i.e., the cross point of the two dispersion surfaces, and so the residue integrals around \( A_1 \) and \( A_4 \) may be neglected. With respect the remained points \( A_2 \) and \( A_3 \), only one of them, \( A_3 \), as indicated in Fig. 3, should be chosen depending on the value of \( K_i \), which gives the energy flow of the crystal wave in the direction lower to the surface. This means that the \( \kappa_z \) root given by \( A_3 \) has a positive imaginary part, and, on the other hand, that given by \( A_2 \) has a negative one. Therefore, the residue integral around \( A_2 \) disappears and only the point \( A_3 \) contributes the integral, because in the integral equation (21) \( r \) is any point in the crystal and \( r' \) is a point on the surface and so \( (z - z') > 0 \) is assumed in the equation. Let the root given to be referred as \( \kappa_y(K_y) \), i.e., a function of \( K_y \), where \( \kappa_y \) is the component of \( \kappa \) parallel to the surface. Furthermore, let the following function be introduced:

\[
f_{bay}^\mu(K_i, \kappa_z(K_i)) = \lim_{\kappa_z \rightarrow \kappa_y(K_y)} \{ \frac{G_{bay}^\mu(K_i, \kappa_z) \cdot (\kappa_z - \kappa_y(K_y))}{(2\pi)^2} \}
\]

Integrating eq. (A1) with respect to \( \kappa_z \) and using equation (A2), equation (A1) is reduced to

\[
G_{gg}^{(t)}(r, r') = \sum_{\mu=1}^{2} \int \int f_{bay}^\mu(K) e^{iK_1(r_1-r'_1)+iK_2(x-x')iK_3(y-y')} |G_{g}^{(t)}(K)|^2 dK_i \quad (2\pi)^2
\]

where \( \kappa = (K_y, K_z(K_y)) \). Substitution of (A3) into eq. (21) suggests a form of the solution

\[
E_g(r) = \sum_{\mu=1}^{2} \int E_g^{(t)}(K) e^{iK_1r_1+iK_2x+iK_3y}|G_{g}^{(t)}(K)|^2 dK_i \quad (2\pi)^2
\]

Using eqs. (A3) and (A4), it may easily be shown that

\[
\int \frac{\partial G_{gg}^{(t)}(r, r')}{\partial n} E_g dS' = \int \frac{\partial G_{gg}^{(t)}(r, r')}{\partial z} E_g dS' = \int G_{gg}^{(t)} \frac{\partial E_g}{\partial z} dS' = - \int G_{gg}^{(t)} \frac{\partial E_g}{\partial z'} dS',
\]

where \( dS' = dx'dy' \) and \( \Gamma_1 \) is the crystal surface with infinite size. Therefore, equation (21) is reduced to

\[
E_g(r) = 2 \int \frac{\partial G_{gg}^{(t)}(r, r')}{\partial z} E_g^{(t)}(r') dS' + 2 \int \frac{\partial G_{gh}^{(t)}(r, r')}{\partial z'} E_h(r') dS', \quad g = 0, h.
\]

Next, we will show a relation about the second term on the right-hand side of eq. (A5) as follows:

\[
\int \frac{\partial G_{gh}^{(t)}(r, r')}{\partial z'} E_h(r') dS' = - \frac{1}{k^2 X_0} \int \left( \left( \frac{\partial G_{gh}^{(t)}(r, r')}{\partial z'} e^{ikr'r'} \right) E_0(r') dS' \right)
\]

This equation may be proved in the following. First, let the integral on the left-hand side of eq. (A6) to be \( I_1 \). Using eqs. (A3) and (A4), the integral on the left-hand side is rewritten to
\[ I_1 = \sum_{\mu=1}^{\frac{3}{2}} \int \left( -iK_{\text{hz}} \right) f_{gh}^{(\mu)}(\kappa) E_{\nu}^{(\mu)}(\kappa) e^{i\kappa_1 r_1 + i\kappa_2 (\kappa_1 x + i\kappa_2 \tau)} e_{\gamma}^{(\mu)}(\kappa) \right) \frac{dK_1}{(2\pi)^2}, \]

where \( \kappa = (\kappa_x, \kappa_z, \kappa_h) \) and \( K_{\text{hz}} = k_{\text{hz}} + h_x + \kappa_z(\kappa_h) \). Furthermore, using the first equation of eq. (23), \( I_1 \) becomes

\[ I_1 = -\sum_{\mu=1}^{\frac{3}{2}} \int \frac{1}{C_{\mu}} \left( -iK_{\text{hz}} \right) f_{gh}^{(\mu)}(\kappa) \left( k^2 (1 + X_0) - K^2 \right) E_{\nu}^{(\mu)}(\kappa) e^{i\kappa_1 r_1 + i\kappa_2 (\kappa_1 x + i\kappa_2 \tau)} e_{\gamma}^{(\mu)}(\kappa) \right) \frac{dK_1}{(2\pi)^2}. \]

On the other hand, with respect to the right-hand side of eq. (A6), using eq. (A2) and integration eq. (43) about \( \kappa_x \) derives

\[ G_{\nu}(r, r') = \sum_{\mu=1}^{\frac{3}{2}} \int \frac{1}{C_{\mu}} \left( -iK_{\text{hz}} \right) f_{gh}^{(\mu)}(\kappa) e^{i\kappa_1 (r_1 - r_1') + i\kappa_2 (\kappa_1 (x - x') + i\kappa_2 \tau - i\kappa_2 \tau')} e_{\gamma}^{(\mu)}(\kappa) \right) \frac{dK_1}{(2\pi)^2}, \]

where \( \kappa = (\kappa_x, \kappa_z, \kappa_h) \). Therefore, if we use eqs. (A4) and (A7), the right-hand side term of eq. (A6), \( I_2 \), becomes

\[ I_2 = -\sum_{\mu=1}^{\frac{3}{2}} \int \frac{1}{C_{\mu}} \left( k^2 (1 + X_0) - K^2 \right) \left( -iK_{\text{hz}} \right) f_{gh}^{(\mu)}(\kappa) E_{\nu}^{(\mu)}(\kappa) e^{i\kappa_1 r_1 + i\kappa_2 (\kappa_1 x + i\kappa_2 \tau)} e_{\gamma}^{(\mu)}(\kappa) \right) \frac{dK_1}{(2\pi)^2}. \]

Therefore, \( I_1 = I_2 \), and so the equation (A6) is justified. Finally, substituting eq. (A6) into eq. (A5) and using the boundary condition \( E_{\gamma}(r') = E_{\gamma}^{(\nu)}(r') \), equation (A5) becomes eq. (42).

References


(平成27年3月31日受理)