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X-ray diffraction from an atomic plane

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Reflection and transmission coefficients of X-rays by a single atomic plane are obtained in the general case where the plane consists of any two-dimensional Bravais lattice and the incident and exit X-ray beams take any direction with respect to the plane. A formula obtained for the coefficients is written in a simple form, different from that obtained by Durbin [*Acta Cryst.* (1995), A**51**, 258–268]. This makes it possible to extend Darwin's dynamical theory of X-ray diffraction to general geometries which include the cases of asymmetric skew reflection and noncoplanar multibeam diffraction.

1. Introduction

Since the advent of synchrotron-radiation sources, X-ray diffraction has been widely used for studying atomic structures of crystal surfaces (Eisenberger & Marra, 1981; Als-Nielsen *et al.*, 1982; Robinson, 1986, 1991; Takahashi *et al.*, 1987; Feidenhans'l, 1989;). In comparison to techniques using electron diffraction, which also provides much information on surface structures, X-ray diffraction allows clear and accurate interpretation of observed intensity data because the data can usually be reproduced by the kinematical theory. However, dynamical treatment is required if multiple diffraction in a crystal cannot be neglected, for example, in the case of grazing-incidence geometry (Kishino & Kohra, 1971; Afanas'ev & Melkonyan, 1983, 1990; Jach *et al.*, 1989; Stepanov *et al.*, 1996) or close to a Bragg point (Taupin, 1964; Halliwell *et al.*, 1984).

The dynamical theory proposed by Darwin (1914) is the first work in which multiple diffraction of X-rays in a perfect crystal is discussed. By decomposing a perfect crystal into a set of single atomic planes parallel to the surface and considering multiple diffraction among them, Darwin obtained a well known profile for symmetrical Bragg reflection, 'the Darwin curve'. Recently, Darwin's theory has attracted attention again because the theory can be applied to calculations not only for Bragg reflection but for CTR (crystal truncation rod) scattering (Caticha, 1994; Nakatani & Takahashi, 1994; Takahashi & Nakatani, 1995; Durbin & Follis, 1995; Chung & Durbin, 1995; Li *et al.*, 1997). Moreover, the theory is of practical use for surface X-ray diffraction. It can be rewritten in the form of a transfer matrix whose elements are made up of transmission and reflection coefficients of a single atomic plane. The diffraction process in a crystal whose surface is different from the substrate is simply described by the product of such matrices. However, most calculations on Darwin's theory that have so far been reported are limited to the case where the scattering plane is perpendicular to the crystal surface.

In the present paper, we extract a formula for the coefficients in general geometry: any two-dimensional Bravais lattice and any direction of incident and exit X-rays. The result shows that the formula is written in a simple form similar to that of Borie (1967), different from the result obtained by Durbin (1995). This allows one to extend Darwin's dynamical theory to general geometries which include the cases of asymmetric skew reflection and noncoplanar multibeam diffraction.

2. Reflection from an atomic plane

In Darwin's theory, one has to obtain the transmission and reflection coefficients by a single atomic plane. Darwin obtained formulae for the coefficients only in the symmetric Bragg case (Darwin, 1914). Borie extended Darwin's theory to the symmetric Laue case (Borie, 1966) and even to the asymmetric Laue case (Borie, 1967). In his paper in 1967, Borie assumed that the atomic plane consists of a square lattice in obtaining simple formulae for the asymmetric case, which can be easily applied to the asymmetric Bragg case (Warren, 1969). However, in all these papers, the scattering vector was assumed to be in the plane perpendicular to the crystal surface. Recently, Durbin has obtained a formulae that can be used even in the symmetric skew reflections from an atomic plane – where the scattering plane is not perpendicular to the crystal surface and the directions of incident and exit waves are symmetric with respect to one of the unit-cell vectors in the plane (Durbin, 1995). He also assumed the same condition that Borie did. Durbin used an approximation in obtaining the formulae, but the result is not so simple as that obtained by Borie.

Here, we extract a formula without using the approximation for the coefficients in general geometry: any two-dimensional Bravais lattice and any direction of incident and exit X-rays.

The resulting formula is written in a simple form which is consistent with Borie's.

We consider the reflection from a single atomic plane shown in Fig. 1 in which the two-dimensional unit cell is defined by unit-cell vectors $\mathbf{a}_1$ and $\mathbf{a}_2$. Here, $\mathbf{a}_1$ and $\mathbf{a}_2$ can be allowed to be in any direction in the atomic plane except that they are parallel to each other. For simplicity, we assume that the unit cell contains only one atom; this assumption is not necessary – we can easily extend the following discussion to the case where more than one atom is contained in the unit cell.

Now let us obtain the formula for the electric field amplitude at an observation point P shown in Fig. 1 when a plane wave of X-rays expressed by a wave vector $\mathbf{k}_0$ ($|\mathbf{k}_0| \equiv 1/\lambda$, λ being the wavelength) irradiates the atomic plane. Here we assume the incident wave is linearly polarized. The plane wave incident on the atomic plane is elastically scattered by the atoms, each of which coherently generates a spherical wave. At the point P, the amplitude of the spherical wave from each atom is given as follows:

$$Cr_e f(\Theta) \exp(-2\pi ikr)/r. \tag{1}$$

Here, C is the polarization factor, r_e is the classical electron radius, r is the distance from each atom generating the spherical wave to P and k is the wave number of the scattered wave ($k \equiv 1/\lambda$). The factor $f(\Theta)$ is the atomic scattering factor (Θ being the scattering angle) given for X-rays. When more than one atom is contained in the unit cell, the atomic scattering factor f is replaced by the crystal structure factor F. We neglect the Debye–Waller factor for simplicity. We define $\mathbf{k}_H$ by a vector parallel to $\overrightarrow{OP}$ whose modulus is $1/\lambda$, *i.e.* $|\mathbf{k}_H| = 1/\lambda$, expressing a diffracted wave. Here, the point O is the origin of the atomic plane, shown in Fig. 1. The origin is defined so that the diffracted wave goes towards the point P.

In order to obtain the total scattering amplitude at the point P, we get the phase difference between the wave passing through O and that passing through any lattice point S in the atomic plane. We divide the total path into two parts, that is, the path for the incident wave and that for the scattered wave. The phase difference for the incident plane wave between the two paths is given as follows:

$$-2\pi \mathbf{k}_0 \cdot (m\mathbf{a}_1 + n\mathbf{a}_2), \tag{2}$$

where m, n are integers, from which $\overrightarrow{OS}$ is expressed by $m\mathbf{a}_1 + n\mathbf{a}_2$. Similarly, the phase difference for the scattered spherical waves is given by

$$-2\pi k(r_{m,n} - r_H), \tag{3}$$

where $r_{m,n} \equiv |\overrightarrow{SP}|$ and $r_H \equiv |\overrightarrow{OP}|$. Since the point P is sufficiently far from the atomic plane, we can assume $ma_1/r_H \ll 1$ and $na_2/r_H \ll 1$. Then we can approximately reduce $r_{m,n}$, neglecting the terms higher than second order, to the following:

$$r_{m,n} = |\mathbf{r}_H - (m\mathbf{a}_1 + n\mathbf{a}_2)| \tag{4}$$

$$= [r_H^2 - 2\mathbf{r}_H \cdot (m\mathbf{a}_1 + n\mathbf{a}_2) + |m\mathbf{a}_1 + n\mathbf{a}_2|^2]^{1/2} \tag{5}$$

$$\approx r_H - \mathbf{s}_H \cdot (m\mathbf{a}_1 + n\mathbf{a}_2) + |m\mathbf{a}_1 + n\mathbf{a}_2|^2 - [\mathbf{s}_H \cdot (m\mathbf{a}_1 + n\mathbf{a}_2)]^2/2r_H, \tag{6}$$

where $\mathbf{s}_H$ is the unit vector parallel to $\mathbf{k}_H$ (or $\mathbf{r}_H$). Thus, from (3) and (6), the phase difference for the scattered waves is rewritten as

$$-2\pi\big(-\mathbf{k}_H \cdot (m\mathbf{a}_1 + n\mathbf{a}_2) + k\{|m\mathbf{a}_1 + n\mathbf{a}_2|^2 - [\mathbf{s}_H \cdot (m\mathbf{a}_1 + n\mathbf{a}_2)]^2\}/2r_H\big). \tag{7}$$

From (2) and (7), the total phase difference $-2\pi\Delta(m, n)$ between the path *via* O and that *via* S is

$$-2\pi\Delta(m,n) = -2\pi\big((\mathbf{k}_0 - \mathbf{k}_H) \cdot (m\mathbf{a}_1 + n\mathbf{a}_2) + k\{|m\mathbf{a}_1 + n\mathbf{a}_2|^2 - [\mathbf{s}_H \cdot (m\mathbf{a}_1 + n\mathbf{a}_2)]^2\}/2r_H\big). \tag{8}$$

With the two-dimensional Bragg condition, the first term in (8) is reduced to zero, therefore we have to take only the second term into account.

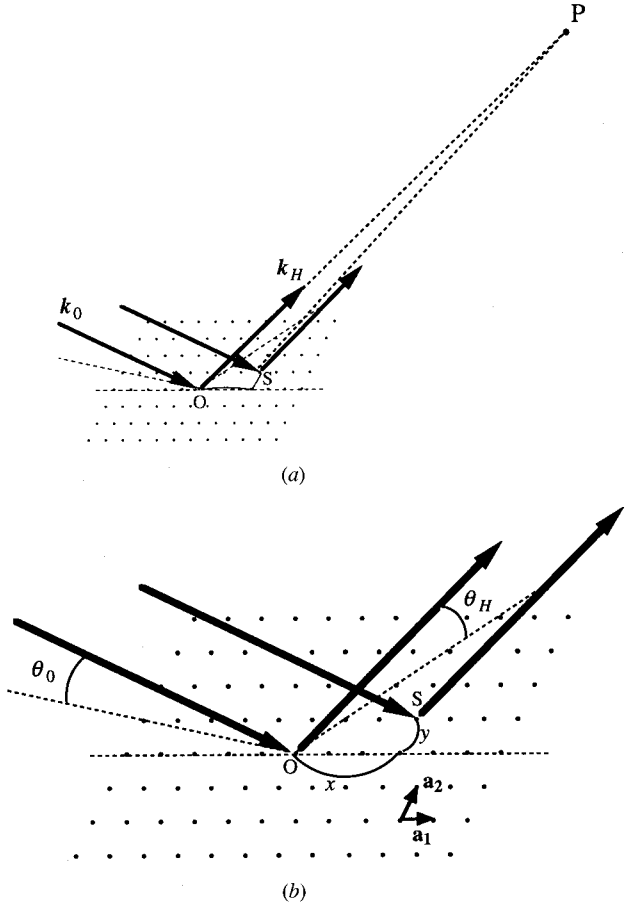

Figure 1
The diffraction from a single atomic plane. (*a*) A bird's-eye view. The vectors $\mathbf{k}_0$, $\mathbf{k}_H$ represent the wave vectors defining the incident and scattered waves, respectively. The point P is the detecting point. (*b*) An enlarged view around the origin O. The vectors $\mathbf{a}_1$, $\mathbf{a}_2$ are unit-cell vectors which define the two-dimensional unit cell in the plane. Waves scattered from all atoms interfere and make a wavefield at the point P.

Next, we integrate the scattered amplitudes from all atoms constituting the plane to obtain the amplitude of the electric field at P. Since the dimensions of the unit cell are sufficiently small compared to r_H, we can treat $m|\mathbf{a}_1|$ ($\equiv x$) and $n|\mathbf{a}_2|$ ($\equiv y$) as continuous values. Then the amplitude $\mathrm{d}E_P$ from an infinitesimal area at (x, y) in the atomic plane is given by

$$\mathrm{d}E_P = -(CMr_e f/r_H)E_0 \exp\{-2\pi i[k(-ct + r_H) + \Delta(m, n)]\} \times |\hat{\mathbf{a}}_1 \times \hat{\mathbf{a}}_2|\,\mathrm{d}x\,\mathrm{d}y. \quad (9)$$

Here, M is the number of unit cells per unit area, given by

$$M = 1/|\mathbf{a}_1 \times \mathbf{a}_2|, \quad (10)$$

and $\hat{\mathbf{a}}_1$ and $\hat{\mathbf{a}}_2$ are unit vectors parallel to $\mathbf{a}_1$ and $\mathbf{a}_2$, respectively. Hence, the total amplitude E_P from all the atoms in the plane is obtained as follows:

$$\begin{aligned} E_P &= \iint_{\text{atomic plane}} \mathrm{d}E_P \\ &= -(CMr_e f/r_H)E_0 \exp[-2\pi ik(-ct + r_H)]|\hat{\mathbf{a}}_1 \times \hat{\mathbf{a}}_2| \\ &\quad \times \iint \exp[-2\pi i\Delta(m, n)]\,\mathrm{d}x\,\mathrm{d}y. \end{aligned} \quad (11)$$

The integral in the second expression of (11) is the well known 'Fresnel integral'; if the integral region is sufficiently large, the integral is reduced to the following:

$$\iint \exp[-2\pi i\Delta(m, n)]\,\mathrm{d}x\,\mathrm{d}y = -i\lambda r_H \Sigma, \quad (12)$$

where Σ is given by

$$\begin{aligned} \Sigma \equiv \{&[1 - (\mathbf{s}_H \cdot \hat{\mathbf{a}}_1)^2][1 - (\mathbf{s}_H \cdot \hat{\mathbf{a}}_2)^2] \\ &- [(\hat{\mathbf{a}}_1 \cdot \hat{\mathbf{a}}_2) - (\mathbf{s}_H \cdot \hat{\mathbf{a}}_1)(\mathbf{s}_H \cdot \hat{\mathbf{a}}_2)]^2\}^{-1/2} \end{aligned} \quad (13)$$

(see Appendix A). Hence, from equations (11), (12) and (13), E_P is rewritten as

$$E_P = -iqE_0 \exp[2\pi ik(-ct + r_H)], \quad (14)$$

where q is defined by

$$q \equiv -CMr_e f\lambda|\hat{\mathbf{a}}_1 \times \hat{\mathbf{a}}_2|\Sigma. \quad (15)$$

The factor q corresponds to the reflection coefficient which was described above. It is worth noting that the diffracted-wave amplitude E_P given by (14) is independent of the distance r_H, that is, the diffracted wave should be regarded as a 'plane wave'.

The above discussion is similar to that of Durbin, although he assumed symmetric skew reflection and a square lattice. However, he reduced a factor equivalent to Σ given by (13) to an approximate form, which is a physically not easily understandable form as is given in Appendix B. In the following discussion, we get a simpler result without further approximations.

Here we use a familiar formula in vector analysis:

$$|\mathbf{a} \times \mathbf{b}|^2 = |\mathbf{a}|^2|\mathbf{b}|^2 - (\mathbf{a} \cdot \mathbf{b})^2. \quad (16)$$

Substituting $\hat{\mathbf{a}}_1 - (\hat{\mathbf{a}}_1 \cdot \mathbf{s}_H)\mathbf{s}_H$ and $\hat{\mathbf{a}}_2 - (\hat{\mathbf{a}}_2 \cdot \mathbf{s}_H)\mathbf{s}_H$ into $\mathbf{a}$ and $\mathbf{b}$ in (16), we get the following relation:

$$\begin{aligned} &|[\hat{\mathbf{a}}_1 - (\hat{\mathbf{a}}_1 \cdot \mathbf{s}_H)\mathbf{s}_H] \times [\hat{\mathbf{a}}_2 - (\hat{\mathbf{a}}_2 \cdot \mathbf{s}_H)\mathbf{s}_H]|^2 \quad (17) \\ &\quad = |\hat{\mathbf{a}}_1 - (\hat{\mathbf{a}}_1 \cdot \mathbf{s}_H)\mathbf{s}_H|^2|\hat{\mathbf{a}}_2 - (\hat{\mathbf{a}}_2 \cdot \mathbf{s}_H)\mathbf{s}_H|^2 \\ &\qquad - \{[\hat{\mathbf{a}}_1 - (\hat{\mathbf{a}}_1 \cdot \mathbf{s}_H)\mathbf{s}_H] \cdot [\hat{\mathbf{a}}_2 - (\hat{\mathbf{a}}_2 \cdot \mathbf{s}_H)\mathbf{s}_H]\}^2 \\ &\quad = [1 - (\mathbf{s}_H \cdot \hat{\mathbf{a}}_1)^2][1 - (\mathbf{s}_H \cdot \hat{\mathbf{a}}_2)^2] \\ &\qquad - [(\hat{\mathbf{a}}_1 \cdot \hat{\mathbf{a}}_2) - (\mathbf{s}_H \cdot \hat{\mathbf{a}}_1)(\mathbf{s}_H \cdot \hat{\mathbf{a}}_2)]^2. \quad (18) \end{aligned}$$

Thus, from (13) and (17), we can rewrite Σ in the form

$$\Sigma = |[\hat{\mathbf{a}}_1 - (\hat{\mathbf{a}}_1 \cdot \mathbf{s}_H)\mathbf{s}_H] \times [\hat{\mathbf{a}}_2 - (\hat{\mathbf{a}}_2 \cdot \mathbf{s}_H)\mathbf{s}_H]|^{-1}. \quad (19)$$

In fact, $\hat{\mathbf{a}}_1 - (\hat{\mathbf{a}}_1 \cdot \mathbf{s}_H)\mathbf{s}_H$ and $\hat{\mathbf{a}}_2 - (\hat{\mathbf{a}}_2 \cdot \mathbf{s}_H)\mathbf{s}_H$ are, respectively, the projections of $\hat{\mathbf{a}}_1$ and $\hat{\mathbf{a}}_2$ into the plane perpendicular to $\mathbf{k}_H$. Thereby, $|[\hat{\mathbf{a}}_1 - (\hat{\mathbf{a}}_1 \cdot \mathbf{s}_H)\mathbf{s}_H] \times [\hat{\mathbf{a}}_2 - (\hat{\mathbf{a}}_2 \cdot \mathbf{s}_H)\mathbf{s}_H]|$ is the projection of the parallelogram defined by $\hat{\mathbf{a}}_1$ and $\hat{\mathbf{a}}_2$ into the plane perpendicular to $\mathbf{k}_H$. Hence, defining θ_H as the angle between $\mathbf{s}_H$ and the atomic plane, we get the following relation:

$$\sin\theta_H = |[\hat{\mathbf{a}}_1 - (\hat{\mathbf{a}}_1 \cdot \mathbf{s}_H)\mathbf{s}_H] \times [\hat{\mathbf{a}}_2 - (\hat{\mathbf{a}}_2 \cdot \mathbf{s}_H)\mathbf{s}_H]|/|\hat{\mathbf{a}}_1 \times \hat{\mathbf{a}}_2|. \quad (20)$$

Consequently, from (15), (19) and (20), we get a simple formula for the coefficient:

$$q_H = -CMr_e f\lambda/\sin\theta_H. \quad (21)$$

This result is consistent with that obtained by Borie. The transmission coefficient q_0 in general geometry is also extracted by the same procedure.

3. Discussion

Applying our result to Darwin's theory, we can obtain reflectivities and transmissivities by a crystal in any geometry – we can assume any Bravais lattice and any direction of incident or exit X-rays. In the two-beam approximation, we can easily extend the result obtained by Takahashi & Nakatani (1995) even to the case where the scattering plane is not perpendicular to the crystal surface, as shown in Fig. 2. In fact, using q given by (21), we can write the reflection and transmission coefficients from a single plane in the same form as theirs:

$$\begin{aligned} t_0 &= 1 - iq_0, \\ r_H &= -iq_H, \end{aligned} \quad (22)$$

where

$$\begin{aligned} q_0 &= -Mr_e f(0)\lambda/\gamma_0, \\ q_H &= -CMr_e f(\Theta_H)\lambda/\gamma_H \end{aligned} \quad (23)$$

and

$$\gamma_0 \equiv \sin\theta_0, \quad (24)$$

$$\gamma_H \equiv \sin\theta_H. \quad (25)$$

The angle Θ_H is defined in Fig. 2. As a result, by means of their method, we can get the absolute reflectivity from a crystal at any point on any reciprocal rod.

For example, the reflection coefficient from a semi-infinite perfect crystal, $R_{H,\infty}$, is given in the same form as the case

where the scattering plane is perpendicular to the crystal surface:

$$\begin{aligned} R_{H,\infty} &= \left(r_H/\{r_H r_{\bar{H}}\ \exp[-i(\varphi_0+\varphi_H)]\}\right)^{1/2}[\eta \pm (\eta^2-1)^{1/2}] \\ &= -|b|^{1/2}(C/|C|)\{F_H/[F_H F_{\bar{H}}\exp(-i2\pi l)]^{1/2}\} \\ &\quad \times [\eta \pm (\eta^2-1)^{1/2}], \end{aligned} \tag{26}$$

where η corresponds to the so-called 'deviation parameter' (Batterman & Cole, 1964), which is defined by

$$\begin{aligned} \eta = \{1 - (t_0 t_H - r_H r_{\bar{H}})\exp[-i(\varphi_0+\varphi_H)]\} \\ \times \left(2\{r_H r_{\bar{H}}\exp[-i(\varphi_0+\varphi_H)]\}^{1/2}\right)^{-1}. \end{aligned} \tag{27}$$

The variables φ_0, φ_H are the phase retardation of incident and exit waves:

$$\begin{aligned} \varphi_0 &= 2\pi|\,\mathbf{a}_3|/\lambda\gamma_0, \\ \varphi_H &= 2\pi|\,\mathbf{a}_3|/\lambda\gamma_H, \end{aligned} \tag{28}$$

and they are related with the index l designating a point on the rod by $\varphi_0 + \varphi_H = 2\pi l$. Here, $\mathbf{a}_3$ is the unit-cell vector which is defined to be perpendicular to the crystal surface. Note that electric fields of incident and exit waves should be decomposed into directions parallel and perpendicular to the scattering plane defined by these waves.

Expression (26) is correct at any point along any reciprocal rod. Near a Bragg point, it gives the familiar Darwin curve; this result is consistent with that obtained by Laue's dynamical theory in the case of asymmetric skew reflection (Zachariasen, 1967). At a point far from a Bragg reflection angle, reflectivity from a semi-infinite crystal, $P_{H,\infty}$, is written as

$$\frac{P_{H,\infty}}{P_0} = \frac{\lambda^2 C^2}{\gamma_0\gamma_H}\frac{|\,\mathbf{a}_3|^2 r_e{}^2}{V^2}\left|\frac{F_H}{1-\exp(-i2\pi l)}\right|^2. \tag{29}$$

This formula says that, even in general geometry, the absolute CTR scattering intensity can be calculated from the kinematical theory using the same correction factor as that obtained by Takahashi & Nakatani (1995).

Takahashi & Nakatani have shown that the theory can be extended to the coplanar three-beam case where the scattering plane is perpendicular to the crystal surface (Takahashi & Nakatani, 1995). However, if the electric field is decomposed in the same manner as the two-beam case, their calculation is also correct even in the case where the scattering plane is *not* perpendicular to the surface.

Furthermore, we can extend the Darwin theory to the *noncoplanar* multibeam case. Near the Bragg points, using the formulae obtained in the present paper, one can show analytically that the Darwin theory is equivalent to the Laue theory for the noncoplanar multiwave Bragg reflection from a semi-infinite perfect crystal (Chang, 1984) if the directions of the incident and all the exit waves take a sufficiently large angle compared to the critical angle of total reflection. It is worth noting that Darwin's original theory is not available for cases when the incident and/or exit waves make angles less than several times the critical angle. The extension of Darwin's theory to such cases is discussed elsewhere.

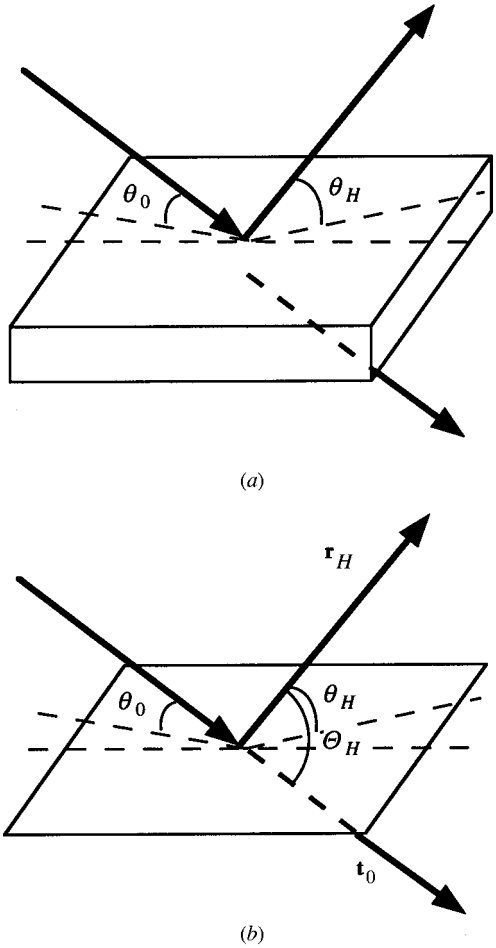

Figure 2
(*a*) Reflection and transmission by a crystal in general geometry. In Darwin's theory, a crystal is divided into atomic planes parallel to the crystal surface. (*b*) The definitions of transmission and reflection coefficients from a single atomic plane.

4. Conclusions

We obtained a simple formula for reflection and transmission coefficients by a single atomic plane in general geometry. The formula (21) obtained by us is similar to that obtained by Borie (1967). This makes it possible to extend Darwin's dynamical theory of X-ray diffraction (Takahashi & Nakatani, 1995) to more general arrangements such as asymmetric skew reflection and noncoplanar multibeam diffraction.

APPENDIX *A*
Calculation of the Fresnel integral

In order to calculate the Fresnel integral in equations (13) and (36), we used the following relation:

$$\begin{aligned} \iint \exp[-2\pi i A(ax^2+2bxy+dy^2)]\,dx\,dy \\ = -i/[2A(ad-b^2)^{1/2}], \end{aligned} \tag{30}$$

which is easily obtained using

$$\iint \exp[-2\pi i(x'^2 + y'^2)]\,\mathrm{d}x'\,\mathrm{d}y' = (1-i)^2 \quad (31)$$

$$= -2i. \quad (32)$$

APPENDIX *B*
Comparison with the formula obtained by Durbin

Durbin gives an approximate formula for symmetric skew reflection from an atomic plane (Durbin, 1995). His formula can be obtained from our rigorous formulae shown in §2. In our notation, the approximate equation (*B*7) in Durbin's paper corresponds to the following:

$$\Delta(m,n) \approx \frac{k\left\{|m\mathbf{a}_1 + n\mathbf{a}_2|^2 - [m^2(\mathbf{s}_H\cdot\mathbf{a}_1)^2 + n^2(\mathbf{s}_H\cdot\mathbf{a}_2)^2]\right\}}{2r_H} \quad (33)$$

$$= \frac{k\left\{x^2[1-(\mathbf{s}_H\cdot\hat{\mathbf{a}}_1)^2] + y^2[1-(\mathbf{s}_H\cdot\hat{\mathbf{a}}_2)^2] + 2xy(\hat{\mathbf{a}}_1\cdot\hat{\mathbf{a}}_2)\right\}}{2r_H}. \quad (34)$$

If the atomic plane consists of a square lattice, *i.e.* $\mathbf{a}_1\cdot\mathbf{a}_2 = 0$ and $|\mathbf{a}_1| = |\mathbf{a}_2|$, using (34), q is written as follows:

$$q = -\lambda C M r_e f \Sigma, \quad (35)$$

where

$$\Sigma = \{[1-(\mathbf{s}_H\cdot\hat{\mathbf{a}}_1)^2][1-(\mathbf{s}_H\cdot\hat{\mathbf{a}}_2)^2]\}^{-1/2}. \quad (36)$$

Substituting q in the above equation into (14), we can obtain an equation identical to equation (*B*8) in Durbin's paper, which is less simple than our result. In addition, using (21), we can show that the integrated intensities of plane- and spherical-wave models across a finite detector area, which were discussed in Appendix *C* of Durbin (1995), are identical even in our general geometry, whereas he showed this fact only in the case of symmetric reflection.

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