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Bragg reflection and transmission of x-rays induced by the imaginary part of the atomic scattering factor

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Abstract. Formulae for x-ray dynamical Bragg diffraction are derived for a plane-parallel crystal with arbitrary thickness. These formulae are applicable even when the contribution of the real part of the atomic scattering factors to the structure factor vanishes. Based on these formulae, dynamical Bragg reflection and transmission induced only by the imaginary part of the atomic scattering factor are studied in detail.

1. Introduction

The general solution for a perfect plane-parallel crystal was given by Zachariasen in 1945 [1]. In Zachariasen's treatment, for convenience, the structure factor F_h (h is the abbreviation of Miller indices $[hkl]$ of the diffracting lattice plane) is given by

$$F_h = F_{hr} + \mathrm{i}F_{hi} \tag{1}$$

where F_{hr} and F_{hi} are the contributions of the real and imaginary parts of the atomic scattering factors, respectively. Zachariasen dealt with the problem under an additional limitation that the absolute value of $k = F_{hi}/F_{hr}$ (real in non-polar crystals) is much smaller than unity, i.e., absorption is very little. Following Zachariasen's theory, for semi-infinite crystals, Hirsch and Ramachandran (1950) extended the theory to large k [2], and Cole and Stemple (1962) and Fingerland (1971) extended the theory to polar crystals [3, 4]. The theoretical details were discussed by James (1963), Batterman and Cole (1964), Kato (1974), and Pinsker (1978) [5–8].

With x-rays from a tunable synchrotron radiation source, it is possible to make F_{hr} zero for some reflections from monatomic and some compound crystals, for example, the 8 4 4 reflection from a Ge single crystal when the x-ray energy is 2.8 eV below its K-absorption edge [9]. There is also a similar situation in resonance Bragg scattering of γ-quanta [10]. In that limit, the diffraction is induced only by F_{hi}, i.e., by the imaginary part of the atomic scattering factor, and the above theories are not valid, because k and its relevant parameters become infinite. In 1993, Fukamachi and Kawamura dealt with this situation for semi-infinite crystals, for simplicity [11].

In this paper, we give general formulae of x-ray dynamical diffraction including reflection and transmission in the Bragg case. These formulae are applicable even when

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F_{hi} is zero for plane-parallel polar or non-polar crystals with arbitrary thickness. Based on these formulae, the properties of dynamical diffraction are studied in detail at the limit where F_{hr} is zero for the Bragg crystals with arbitrary thickness.

2. Theory

The coherent scattering factor in a crystal is expressed by using the Fourier component of electron susceptibility χ_h in the atomic unit form ($\hbar = m = e = 1$) as

$$\chi_h = \chi_{hr} + \mathrm{i}\chi_{hi} \tag{2}$$

where

$$\chi_{hr} = |\chi_{hr}| \exp(\mathrm{i}\alpha_{hr}) = -(4\pi/v\omega^2)F_{hr} \tag{3}$$

and

$$\chi_{hi} = |\chi_{hi}| \exp(\mathrm{i}\alpha_{hi}) = -(4\pi/v\omega^2)F_{hi}. \tag{4}$$

In (3) and (4), v is the unit cell volume and ω the x-ray energy. The phase difference is given by

$$\delta = \alpha_{hi} - \alpha_{hr}. \tag{5}$$

We write the product of χ_h and χ_{-h} as

$$\chi_h\chi_{-h} = |\chi_h|^2(1 - b^2 + \mathrm{i}\,2p\cos\delta) \tag{6}$$

where

$$|\chi_h|^2 = |\chi_{hr}|^2 + |\chi_{hi}|^2 \qquad b = \sqrt{2}|\chi_{hi}|/|\chi_h|^2$$

and

$$p = |\chi_{hr}||\chi_{hi}|/|\chi_h|^2. \tag{7}$$

In the two-beam approximation [1, 8, 12], the displacement field within the crystal is a Bloch wave of the form

$$D = \mathrm{e}^{-\mathrm{i}\omega t}(D_0\,\mathrm{e}^{\mathrm{i}k_0\cdot r} + D_h\,\mathrm{e}^{\mathrm{i}k_h\cdot r}) \tag{8}$$

where $k_h = k_0 + h$ and the amplitudes satisfy the system of equations

$$2(\xi_0 - \mathrm{i}\kappa_{0i})D_0 - P\chi_h\kappa_{0r}D_h = 0 \tag{9}$$

$$-P\chi_h\kappa_{0r}D_0 + 2(\xi_h - \mathrm{i}\kappa_{0i})D_h = 0 \tag{10}$$

with the resonance defects ξ_0 and ξ_h defined by

$$\xi_0 = k_0 - \kappa_{0r} \tag{11}$$

$$\xi_h = k_h - \kappa_{0r} \tag{12}$$

where $\kappa_{0r} = K(1 + \chi_{0r}/2)$, $\kappa_{0i} = K\chi_{0i}/2$, K is the incident vacuum wave vector and P is the polarization factor. The wave vectors k_0 and k_h are determined by two conditions. The first is that they are constrained to lie on the dispersion surface. This is expressed by

$$(\xi_0 - \mathrm{i}\kappa_{0i})(\xi_h - \mathrm{i}\kappa_{0i}) = \kappa_{0r}^2P^2\chi_h\chi_{-h}/4. \tag{13}$$

The second is that they are related to the incident vacuum wave vector through a tangential continuity boundary condition.

In the following, we consider only the σ-polarization case.The discussion for π-polarization is the same except that we multiply χ_h by P.

The dispersion surface in the two-beam approximation is shown in figure 1, which defines the X and Y axes; the resonance error W, which expresses the degree of deviation from the exact Bragg condition, is given by

$$W = -\frac{X_0 \sin 2\theta}{|\cos\theta_1 \cos\theta_2|^{\frac{1}{2}} \kappa_{0r} |\chi_h|} \tag{14}$$

where θ is the Bragg angle; the parameters X_0, θ_1, θ_2, are shown in figure 1. Note that W defined in this way is applicable to the case in which either χ_{hr} or χ_{hi} is zero [11]. In the Bragg case, $\cos\theta_2 < 0$.

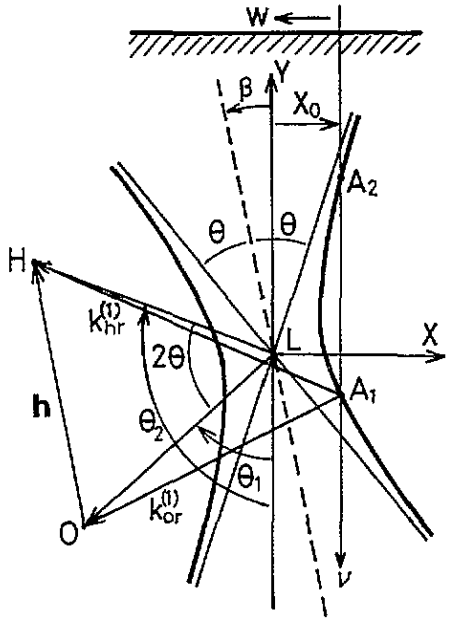

Figure 1. Schematic diagram of the dispersion surface. The origin of the reciprocal vector is O, the diffraction point is H and the Laue point is L. Axis X is parallel to the crystal surface.

From (13), using coordinate transformation [12], we can get the values of Y_0 for excitation points A_1 and A_2:

$$Y_0 = \frac{-\kappa_{0r}|\chi_h|}{2|\cos\theta_1 \cos\theta_2|^{\frac{1}{2}}} \left\{ W \frac{\sin 2\beta}{\sin 2\theta} + \mathrm{i}g \frac{\cos\theta \sin\beta}{|\cos\theta_1 \cos\theta_2|^{\frac{1}{2}}} \right.$$
$$\left. \pm [(W + \mathrm{i}g')^2 - (1 - b^2 + \mathrm{i}\,2p\cos\delta)]^{\frac{1}{2}} \right\} \tag{15}$$

where

$$g = \frac{\chi_{0i}}{|\chi_h|} \tag{16}$$

$$g' = g(\sin\theta\cos\beta)/|\cos\theta_1 \cos\theta_2|^{\frac{1}{2}} \tag{17}$$

so we have

$$\xi_0^{(1,2)} - \mathrm{i}\kappa_{0i} = (X_0 \sin\theta_1 + Y_0 \cos\theta_1) - \mathrm{i}g\kappa_{0r}|\chi_h|/2$$

$$= \frac{1}{2}k_{0r}|\chi_h|\left|\frac{\cos\theta_1}{\cos\theta_2}\right|^{\frac{1}{2}}\{-(W+\mathrm{i}g') \pm[(W+\mathrm{i}g')^2-(1-b^2+\mathrm{i}2p\cos\delta)]^{\frac{1}{2}}\}. \tag{18}$$

According to (9)–(13), we have

$$r_1 = D_h^{(1)}/D_0^{(2)} = 2(\xi_0^{(1)} - \mathrm{i}\kappa_{0i})/(\chi_{-h}\kappa_{0r})$$
$$= \frac{|\chi_h|}{\chi_{-h}}\left|\frac{\cos\theta_1}{\cos\theta_2}\right|^{\frac{1}{2}}\{-(W+\mathrm{i}g') + [(W+\mathrm{i}g')^2-(1-b^2+\mathrm{i}2p\cos\delta)]^{\frac{1}{2}}\} \tag{19}$$

$$r_2 = D_h^{(2)}/D_0^{(2)} = 2(\xi_0^{(2)} - \mathrm{i}\kappa_{0i})/(\chi_{-h}\kappa_{0r})$$
$$= \frac{|\chi_h|}{\chi_{-h}}\left|\frac{\cos\theta_1}{\cos\theta_2}\right|^{\frac{1}{2}}\{-(W+\mathrm{i}g') - [(W+\mathrm{i}g')^2-(1-b^2+\mathrm{i}2p\cos\delta)]^{\frac{1}{2}}\}. \tag{20}$$

The boundary conditions on the entrance surface are

$$D_0^{(1)} + D_0^{(2)} = E_0^a \tag{21}$$

$$D_h^{(1)} + D_h^{(2)} = E_h^a. \tag{22}$$

The conditions on the exit surface are

$$D_0^{(1)}\,\mathrm{e}^{-2\pi\mathrm{i}k_{0z}^{(1)}H} + D_0^{(2)}\,\mathrm{e}^{-2\pi\mathrm{i}k_{0z}^{(2)}H} = E_d\,\mathrm{e}^{-2\pi\mathrm{i}K_{0z}H} \tag{23}$$

$$D_h^{(1)}\,\mathrm{e}^{-2\pi\mathrm{i}k_{hz}^{(1)}H} + D_h^{(2)}\,\mathrm{e}^{-2\pi\mathrm{i}k_{hz}^{(2)}H} = 0. \tag{24}$$

In (21)–(24), E_h^a is the amplitude of the wave reflected into the vacuum on the entrance surface, and E_d^a is the amplitude of the wave emerging into the vacuum through the exit surface; H is the crystal thickness. From (19), (20), (21) and (24), we have

$$D_0^{(1)} = \frac{r_2\,\mathrm{e}^{-2\pi\mathrm{i}k_{hz}^{(2)}H}}{r_2\,\mathrm{e}^{-2\pi\mathrm{i}k_{hz}^{(2)}H} - r_1\,\mathrm{e}^{-2\pi\mathrm{i}k_{hz}^{(1)}H}}E_0^a \tag{25}$$

$$D_0^{(2)} = -\frac{r_1\,\mathrm{e}^{-2\pi\mathrm{i}k_{hz}^{(1)}H}}{r_2\,\mathrm{e}^{-2\pi\mathrm{i}k_{hz}^{(2)}H} - r_1\,\mathrm{e}^{-2\pi\mathrm{i}k_{hz}^{(1)}H}}E_0^a. \tag{26}$$

According to (21)–(25), we get

$$\frac{E_h^a}{E_0^a} = \frac{r_1 r_2\left[\mathrm{e}^{-2\pi\mathrm{i}k_{hz}^{(2)}H} - \mathrm{e}^{-2\pi\mathrm{i}k_{hz}^{(1)}H}\right]}{r_2\,\mathrm{e}^{-2\pi\mathrm{i}k_{hz}^{(2)}H} - r_1\,\mathrm{e}^{-2\pi\mathrm{i}k_{hz}^{(1)}H}} \tag{27}$$

$$\frac{E_d^a}{E_0^a} = \frac{r_2\,\mathrm{e}^{-2\pi\mathrm{i}(k_{0z}^{(1)}+k_{hz}^{(2)})H} - r_1\,\mathrm{e}^{-2\pi\mathrm{i}(k_{hz}^{(1)}+k_{0z}^{(2)})H}}{r_2\,\mathrm{e}^{-2\pi\mathrm{i}k_{hz}^{(2)}H} - r_1\,\mathrm{e}^{-2\pi\mathrm{i}k_{hz}^{(1)}H}}. \tag{28}$$

To simplify the intensity formulae, we define

$$g_0 = \chi_{0i}/|\chi_{hi}| \tag{29}$$

$$q = \frac{1}{1+|\chi_{hr}|^2/|\chi_{hi}|^2} \tag{30}$$

$$a = \cos\theta_1/|\cos\theta_2|. \tag{31}$$

In (30), the parameter q is related to x-ray energy and diffracting lattice plane. In (31), a is one parameter that indicates the reflection condition: $a = 1$, $a > 1$ and $a < 1$ represent the symmetric case, negative asymmetry and positive asymmetry, respectively, as shown in

figure 2. The quantities g_0 and g are nonpositive. According to (7), (29), (30) and (31), we get

$$b = (2q)^{1/2} \tag{32}$$

$$p = [q(1-q)]^{1/2} \tag{33}$$

$$g = g_0 q^{1/2}. \tag{34}$$

From (27), the reflectivity, i.e. the ratio of the reflection intensity, P_h, and the incident intensity P_0, is given by

$$\frac{P_h}{P_0} = \left|\frac{E_h^a}{E_0^a}\right|^2 \frac{|\cos\theta_2|}{\cos\theta_1} = \frac{[\cosh(2sHI_1) - \cos(2sHR_1)]P_2}{(1+2p\sin\delta)P_1} \tag{35}$$

where

$$P_2 = [(W+R_1)^2 + (g'+I_1)^2][(W-R_1)^2 + (g'-I_1)^2] \tag{36}$$

$$\begin{aligned} P_1 = {} & \cosh(2sHI_1)(W^2 + g'^2 + R_1^2 + I_1^2) - 2\sinh(2sHI_1)(WR_1 + g'I_1) \\ & - \cos(2sHR_1)(W^2 + g'^2 - R_1^2 - I_1^2) + 2\sin(2sHR_1)(WI_1 - g'R_1) \end{aligned} \tag{37}$$

$$R_1 = \pm[(A + L_1)/2]^{\frac{1}{2}} \tag{38}$$

$$I_1 = \pm[(L_1 - A)/2]^{\frac{1}{2}} \tag{39}$$

$$L_1 = (A^2 + B^2)^{\frac{1}{2}} \tag{40}$$

$$A = W^2 - g'^2 - 1 + b^2 \tag{41}$$

$$B = 2(g'W - p\cos\delta) \tag{42}$$

$$g' = \frac{g(a+1)}{2a^{\frac{1}{2}}}. \tag{43}$$

The parameter s is given by

$$s = \frac{\pi\kappa_{0r}|\chi_h|}{|\cos\theta_1\cos\theta_2|^{\frac{1}{2}}}. \tag{44}$$

In (38), we take the negative sign only when $A < 0$ and $B < 0$, but only when $A > 0$ and $B < 0$ in (39). If the transmitted x-ray intensity is denoted by P_d, from (28), P_d/P_0 is given by

$$\frac{P_d}{P_0} = \left|\frac{E_d^a}{E_0^a}\right|^2 = 2\exp\left[\frac{sHg(a-1)}{a^{1/2}}\right]\frac{L_1}{P_1}. \tag{45}$$

Owing to the factor $2p\sin\delta$ in (35), the reflection intensity P_h/P_0 from the two diffracting lattice planes with h and $-h$ is different for a polar crystal. But in (45), there is no factor $2p\sin\delta$ but $2p\cos\delta$. Since $2p\cos(-\delta) = 2p\cos\delta$, the transmission intensity from the two diffracting lattice planes with h and $-h$ is the same. When $\chi_{hr} = p = 0$, $2p\sin\delta = 2p\sin(-\delta) = 0$, the polarity dependence of the reflection intensity vanishes. The Freidel law holds if $\chi_{hr} = 0$, which is also indicated in [11].

The integral power R in the angle-dispersive mode is given by

$$R = \left|\frac{\cos\theta_1}{\cos\theta_2}\right|^{\frac{1}{2}} \frac{|\chi_h|}{\sin 2\theta}\int \frac{P_x}{P_0}\,\mathrm{d}W \tag{46}$$

where P_x is P_h or P_d. R is a function of a, q, s, H, g_0 and δ.

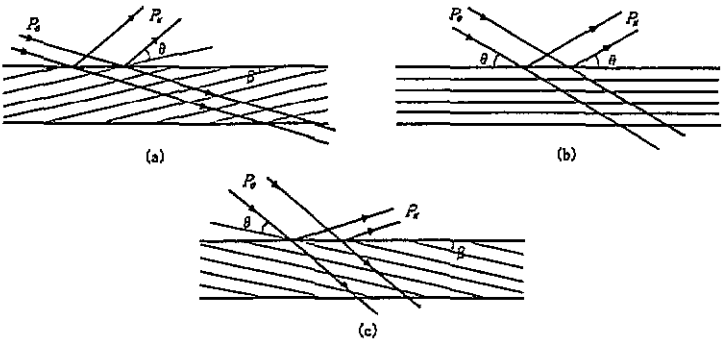

Figure 2. The Bragg scattering geometry for a finite-thickness slab: (a) negative asymmetry $a > 1$, (b) symmetry $a = 1$, (c) positive asymmetry $a < 1$.

3. Bragg reflection and transmission when $\chi_{hr} = 0$

Based on the above formulae, the dynamical diffraction, induced only by the imaginary part of the atomic scattering factor in the Bragg case from a plane-parallel crystal with arbitrary thickness, is studied in detail below.

3.1. Bragg reflection

In figure 3, the reflectivities P_h/P_0 are shown as a function of W defined in (14) from -10 to 10. They are the so-called rocking curves. When $\chi_{hr} = 0$ ($q = 1$), each of them has the maximum value when $W = 0$ and is symmetric with respect to $W = 0$, whether the symmetric reflection condition ($a = 1$) is taken (curves 1, 2) or not (curve 3). But when χ_{hr} is not equal to zero, for example, $|\chi_{hr}| = |\chi_{hi}|$ ($q = 0.5$), the rocking curve is not symmetric with respect to $W = 0$, though $a = 1$ (curve 4). Therefore, the fact that the rocking curve is always symmetric with respect to $W = 0$ is one of the most important characteristics of the dynamical reflection induced by the imaginary part of the atomic scattering factor. This feature is helpful for judging whether the condition $q = 1$ is satisfied or not. When the crystal is thin enough, we can see the *Pendellösung* fringes induced by the imaginary part of the atomic scattering factor (curves 2, 3), as in the Laue case [11]. When $sH = 40$ (curve 1), the crystal can be regarded as infinite, the maximum reaches unity, and the curve is very sharp as indicated by Fukamachi and Kawamura [11]. In this case, there is no gap between the two branches which are tangential to each other at $W = 0$, in the dispersion surface [13].

The integral power $R(sH)$ of the reflected beam in the Bragg case is shown in figure 4, for the case of $q = 1$ and $q = 0.5$. The curves are approximately linear when sH is comparatively small and reach steady values when sH is large. Curve 2 represents the case of a monatomic or centrosymmetric compound crystal. Curve 1 lies under curve 2 because of more absorption. Curves 3 and 4 represent the case of the two diffracting lattice planes with h and $-h$, respectively, for a polar crystal. Their difference is due to crystal polarity. However, curve 1 represents any crystal, because the effect of the crystal polarity disappears when $q = 1$. Figure 5 shows the relationship of the integral power of the reflected beam and the parameter q for a crystal with finite thickness. Curve 1 represents the case of nonpolar crystals. It can be seen that $R(q)$ has the minimum value when $q = 1$. Curves 2 and 3 represent the case of polar crystals. Because both q and δ depend on x-ray energy and diffracting lattice plane, although the different points in curves 2 and 3 have the same value

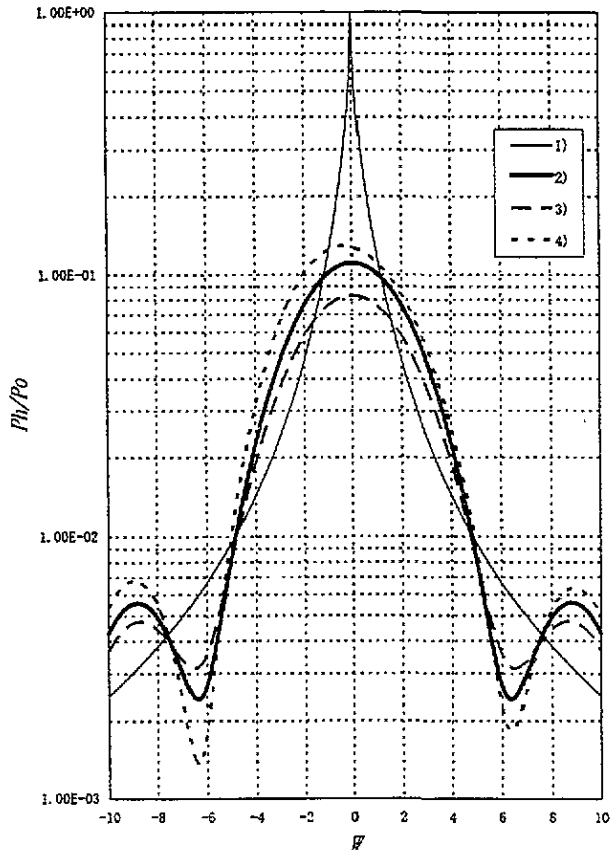

Figure 3. The rocking curves of the diffracted beam in the Bragg case. The parameters are (1) $q = 1, a = 1, sH = 40, g_0 = -1$; (2) $q = 1, a = 1, sH = 0.5, g_0 = -1$; (3) $q = 1, a = 5$ (or 0.2), $sH = 0.5, g_0 = -1$; (4) $\delta = 0, q = 0.5, a = 1, sH = 0.5, g_0 = -1$

of δ, they represent different diffracting lattice planes because of the different values of q. We cannot compare the values in a single curve. Nevertheless, it is worth noting that the two points with the same value of q in curves 2 and 3 represent the two diffracting planes with h and $-h$. Their difference is due to the crystal polarity. They intersect when $q = 1$, which means that Friedel's law holds in this case. Experimentally, we can also use this feature to judge whether the condition of $q = 1$ is satisfied or not.

3.2. Bragg transmission

The rocking curves of the transmitted beam for a plane-parallel crystal in the Bragg case for $q = 1$ (curves 1 to 5) and $q = 0.5$ (curve 6) are shown in figure 6. Their symmetry is the same as that of the reflected beam, but the *Pendellösung* fringes are not found. Curves 1, 2, 3 indicate that, with increasing crystal thickness, the intensity ratio decreases. Curves 3, 4, 5 show the effect of the reflection condition on the intensity of the transmitted beam. When the other parameters are the same, the transmitted intensity is the largest for negative asymmetry ($a > 1$), the smallest for positive asymmetry ($a < 1$). The former is called abnormal transmission.

Figure 7 shows the integral intensity variation of the reflected and transmitted beam as

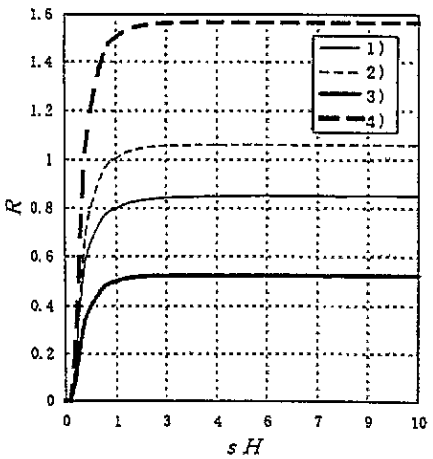

Figure 4. The integral reflecting powers $R(sH)$ of the diffracted beam in the Bragg case. The parameters are $a = 1, g_0 = -1$, (1) $q = 1$; (2) $q = 0.5, \delta = 0$; (3) $q = 0.5, \delta = \pi/6$; (4) $q = 0.5, \delta = -\pi/6$.

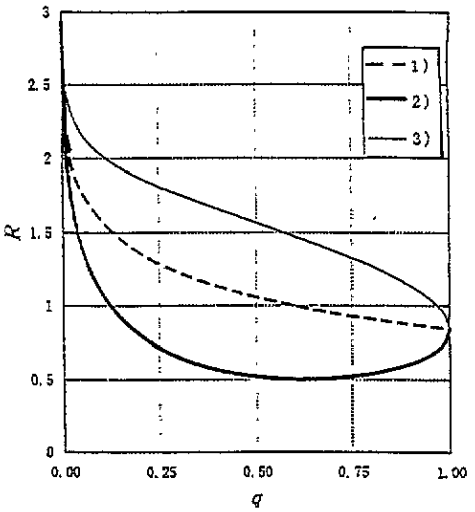

Figure 5. The integral reflecting powers $R(q)$ of the diffracted beam in the Bragg case. The parameters are $a = 1, sH = 3, g_0 = -1$, (1) $\delta = 0$; (2) $\delta = \pi/6$; (3) $\delta = -\pi/6$.

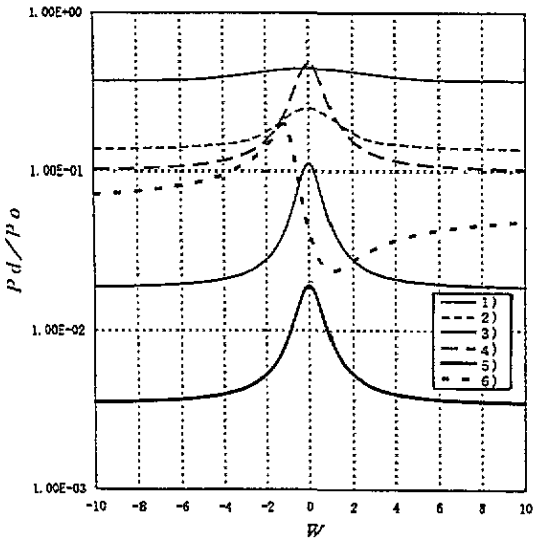

Figure 6. The rocking curves of the transmitted beam in the Bragg case from a plane-parallel crystal. The parameters are $g_0 = -1$; (1) $q = 1, a = 1, sH = 0.5$; (2) $q = 1, a = 1, sH = 1$; (3) $q = 1, a = 1, sH = 2$; (4) $q = 1, a = 3, sH = 2$; (5) $q = 1, a = 0.5, sH = 2$; (6) $\delta = 0, q = 0.5, a = 1, sH = 2$.

a function of the parameter a. For the reflected beam, it changes slowly with the parameter a and is the largest when the symmetric reflection condition is taken. However, for the transmitted beam it is very sensitive to the reflection condition.

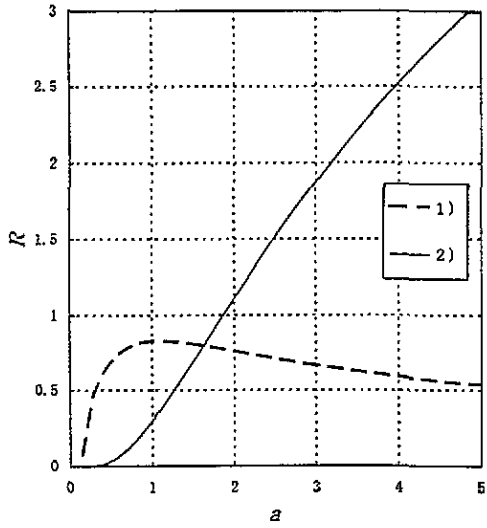

Figure 7. Integral intensity variation of the reflected (curve 1) and transmitted (curve 2) beams as a function of the parameter a. Other parameters are $q = 1, sH = 2, g_0 = -1, \delta = 0$.

4. Summary

We have derived the formulae for x-ray dynamical diffraction intensities for a plane-parallel crystal with arbitrary thickness in the Bragg case. The formulae are applicable not only to the case without absorption, but also to that of strong absorption when diffraction is induced only by the imaginary part of the atomic scattering factors. Based on these formulae, we have discussed the Bragg diffraction induced only by the the imaginary part of the atomic scattering factor for a plane-parallel crystal with arbitrary thickness. The following conclusions have been obtained.

Firstly, the rocking curve is always symmetric with respect to $W = 0$, whether the symmetric reflection condition is taken or not. We found the *Pendellösung* fringes induced by the imaginary part of the atomic scattering factor, when the crystal is thin enough.

Secondly, Friedel's law holds when $\chi_{hr} = 0$, even for a polar finite crystal.

Thirdly, for a monatomic or centrosymmetric compound crystal, the integral reflecting power takes the minimum value when $\chi_{hr} = 0$.

Finally, the transmitted intensity is very sensitive to the reflection condition and increases as the parameter a increases. It is well known that it is very difficult to detect point defects of the order of 1 μm in a nearly perfect crystal by conventional x-ray topography, so the Borrmann effect is used instead. In 1971, Kishino obtained the numerical solutions to the elementary equations in the Bragg case for a thin crystal and pointed out an anomalous enhancement of a transmitted beam at extremely asymmetric reflection [14]. This effect was later used to study the perfection of GaP [15]. We have derived the analytical solutions and obtained the same result more simply than Kishino, so they could be used for x-ray topography based on the Borrman effect more conveniently.

Acknowledgments

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