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DIFFRACTION AND SCATTERING OF IONIZING RADIATIONS

Theory of the Laue Diffraction of X Rays in a Thick Single Crystal with an Inclined Step on the Exit Surface. II: Analytical Solution

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Abstract—The analytical solution of the problem of the Laue diffraction of an X-ray spherical wave in a single crystal with an inclined step on the exit surface has been obtained. The general equations are used for the specific case of plane wave diffraction in a thick crystal under the Borrmann conditions. It is shown that, provided that the crystal thickness increases from the side of the reflected beam, the reflected-wave relative amplitude is determined by three complex terms. This may formally lead to interference and an increase in the intensity in maxima by a factor of 9 as compared with the crystal without a step. The equation for the transmitted beam contains only two terms, and the corresponding increase in intensity cannot be by more than a factor of 4. The results of analytical calculations coincide with the results obtained by numerical methods and presented in the first part of the work.

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INTRODUCTION

In this paper, we report the results of the work the first part of which was published in [1]. The problem of spatial distribution (in the beam cross section) of the intensities of transmitted and reflected waves is solved theoretically for the case of Laue diffraction of X rays in a thick single crystal with an inclined step on its exit surface. This problem was solved numerically in the first part of the work. A significant redistribution of the reflected-beam intensity was observed in the transition region between the step boundary and the boundary of Borrmann triangle with a vertex at the lower step boundary: the intensity maxima increased by a factor of more than 7 in comparison with the intensity before the step. It should also be noted that the transmitted-beam intensity, averaged over the interference region, and the total intensity of the two beams are reduced significantly, which indicates violation of the Borrmann conditions.

It was shown in [1] that the problem can be divided for convenience into two stages. In the first stage, a plate-shaped crystal is under consideration and the solution is found using the Fourier transform method (as was made in [2–6]). In the second stage, one must solve the Takagi equations [7]. If the sample lattice is not strained but the sample shape has a complex boundary, these equations can be solved in the integral form [8–14]. In some cases, the integral form of equations excludes a direct solution to the problem but yields an equation that can sometimes be solved analytically.

Specifically this case is implemented in the problem of Laue diffraction in a single crystal with an inclined step on its exit surface (the object of our consideration). In this paper, we report the results of analytical solution for the second stage of the problem. The method that was first applied in [15] is used.

FORMULATION OF THE PROBLEM AND ITS ANALYTICAL SOLUTION

The schematic of the numerical experiment was reported in the first part of the work. It is assumed that a monochromatic spherical wave from a point X-ray source, located at a distance L from the sample, is incident on a plate-shaped single crystal of thickness t (maximum thickness). There is an inclined step of height t_0 on the exit crystal surface. We assume that the wave functions $E_0(x)$ and $E_h(x)$ for the transmitted and reflected beams, respectively, are known at the thickness $z = t_1 = t - t_0$.

In the second stage, one must solve the Takagi equations [7]

$$\frac{2}{i}\frac{\partial E_0}{\partial s_0} = X_0 E_0 + X_{-h} E_h \exp(i\mathbf{hu}), \quad (1)$$

$$\frac{2}{i}\frac{\partial E_h}{\partial s_h} = [X_0 + 2\alpha_q] E_h + X_h E_0 \exp(-i\mathbf{hu}). \quad (2)$$

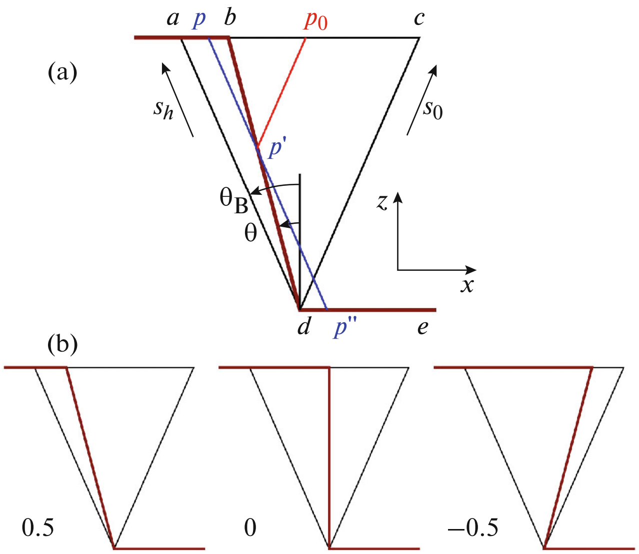

Fig. 1. (a) Exit crystal boundary in the form of step and a Borrmann triangle, in which at least one field depends on the x coordinate. (b) Different versions of step inclination at different values of parameter $R = \tan\theta/\tan\theta_B$ (with indication of the values of parameter R).

Here, $X_{0,h,-h} = K\chi_{0,h,-h}$, where $K = 2\pi/\lambda$ is the wave number; χ_0, χ_h, and χ_{-h} are the Fourier components of the crystal polarizability for the reciprocal-lattice vectors **0**, **h**, and −**h**, respectively; the coordinates s_0 and s_h are counted along the propagation directions of the transmitted and reflected waves, respectively; **u** is the displacement vector due to the possible lattice strain; the parameter of deviation from the Bragg condition is $\alpha_q = K(\theta - \theta_0)\sin 2\theta_B$; and λ is the X-ray wavelength. The angle θ–θ_0 describes the crystal angular position with respect to the incident beam.

Let us consider the case where $\alpha_q = 0$ and there are no strains in the crystal ($\mathbf{u} = 0$). For a perfect crystal, one can solve Eqs. (1) and (2) in the integral form in terms of known fields E_0 and E_h at some boundary in the Borrmann triangle, whose vertex is located at the observation point and sides are oriented along the directions of the transmitted (s_0) and reflected (s_h) waves [8–14]. The case where the thickness t_1 of crystal planar part exceeds greatly the diffraction focusing length [6, 16]: $t_{df} = L|\chi_h|F$, where $F = 1/(\sin\theta_B \sin 2\theta_B)$ and θ_B is the Bragg angle. In this case, the wave function is almost constant on the horizontal x axis in the step region (thickness t_1), which corresponds to plane wave was considered in [1].

In contrast to [1], we will consider the case of a plane wave incident on a crystal, with the Bragg conditions exactly satisfied. The distance between the point source and crystal should be much larger than the diffraction focusing length $L_{df} = t_1C$, where $C = (|\chi_h|F)^{-1}$. For $t_1 = 1$ mm, this length is $L_d = 32.9$ m. Note that the incident beam can easily be collimated on third-generation synchrotron radiation sources using a compound refractive lens [17].

Figure 1a shows the sample shape in the region of step on the exit surface, as well as the Borrmann triangle in which at least one wave function depends on the x coordinate. We apply the approach that was proposed for the first time in [15]. It implies consideration of the difference in the wave functions for the sample under study, $E_k(\mathbf{r})$, and for the plate-shaped sample, $A_k(z)$, rather than the real wave functions. Note that the function $A_k(z)$ for a plane wave is known in the analytical form. Obviously, the integral equations for the differences will be the same; however, the boundary conditions differ significantly, because the difference in the wave functions is zero in the region where the crystal is homogeneous along the x axis.

Thus, we consider the functions

$$e_k(\mathbf{r}) = (E_k(\mathbf{r}) - A_k(z))F_0^{-1}(z), \quad k = 0, h, \tag{3}$$

where

$$A_k(z) = C_k F_0(z) F_h^{-1}(z), \quad F_{0,h} = \exp(iX_{0,h}z/2\gamma_0). \tag{4}$$

Here, $\gamma_0 = \cos\theta_B$ and the coefficients C_k depend on the normalization. For a plane wave, they are equal to ± 0.5 at $k = 0, h$, respectively. Note that the fields $e_k(\mathbf{r})$ are nonzero only in the *acd* triangle (Fig. 1a).

According to the integral formulation of theory [12], the function $e_h(p)$ at a point p on the segment *ab* can be expressed in terms of the functions on the *ad* and *db* lines. Taking into account that the field differences on the *ad* line are zero, we obtain a solution in the form

$$e_h(p) = e_h(p') - \int\limits_{dp'} ds_0 \frac{\partial R}{\partial s_0} e_h - \frac{i}{2} X_h \int\limits_{dp'} ds_h R e_0, \tag{5}$$

$$R = J_0(X((s_{0p} - s_0)(s_{hp} - s_h))^{1/2}), \tag{6}$$

where $X = (X_h X_{-h})^{1/2}$ and s_{0p} and s_{hp} are the coordinates of point p. Hereinafter, we denote the nth-order Bessel function as $J_n(x)$. At the same time, the function $e_0(p')$ on the *db* line is a solution to the integral equation

$$e_0(p') = \int\limits_{dp'} ds_h \frac{\partial R}{\partial s_h} e_0 + \frac{i}{2} X_{-h} \int\limits_{dp'} ds_0 R e_h \tag{7}$$

if the function $e_h(\mathbf{r})$ is known on this line. In the case under consideration, the *db* line is straight. We introduce coordinates ξ and ξ_η for the points on the dp' line and at the point p'. The old and new coordinates are interrelated as follows:

$$z = \cos\theta_B(s_0 + s_h) = \xi\cos\theta, \\ x = \sin\theta_B(s_0 - s_h) = -\xi\sin\theta. \tag{8}$$

Let us denote the argument of the Bessel function in (6) as A. Taking into account (8), one can easily find that, on the *db* line,

$$s_0 = \gamma_1\xi, \quad s_h = \gamma_2\xi,$$
$$A = b(\xi_\eta - \xi), \quad b = X(\gamma_1\gamma_2)^{1/2}, \tag{9}$$

where

$$\xi_\eta = \xi_0 - \eta D_1, \quad \xi_0 = \frac{t_0}{\gamma}, \quad D_1 = \frac{\gamma_0}{\sin(\theta_B - \theta)}, \tag{10}$$

$$\gamma_1 = \frac{\sin(\theta_B - \theta)}{\sin 2\theta_B}, \quad \gamma_2 = \frac{\sin(\theta_B + \theta)}{\sin 2\theta_B}, \quad \gamma = \cos\theta. \tag{11}$$

Here, ξ_η and η are the lengths of segments dp' and pb, respectively. Then we determine the dependence of the intensities of transmitted and reflected waves on the parameter η.

The integral in (7) is calculated over the coordinate ξ in the range from zero to ξ_η. For simplicity, we will make a replacement of variables $\xi \to \xi_\eta - \xi$, which does not change the integration limits. Then the derivative can be written as

$$\frac{\partial R}{\partial s_h} = \frac{1}{2}X\left(\frac{s_0}{s_h}\right)^{1/2} J_1(A) = \frac{1}{2}X\left(\frac{\gamma_1}{\gamma_2}\right)^{1/2} J_1(b\xi). \tag{12}$$

As a result, Eq. (7) takes the following form after the replacement of variables:

$$e_0(\xi_\eta) = \frac{b}{2}\int_0^{\xi_\eta} d\xi e_0(\xi_\eta - \xi)J_1(b\xi) + \frac{i}{2}X_{-h}\gamma_1\int_0^{\xi_\eta} d\xi e_h(\xi_\eta - \xi)J_0(b\xi). \tag{13}$$

On the right-hand side there are integrals in the form of convolutions. Integral equation (13) can be solved applying the Laplace transform

$$e(q) = \int_0^\infty d\xi \exp(-q\xi)e_0(\xi) \tag{14}$$

and using its property, according to which a convolution of two functions is transformed into the product of their transforms. Then we arrive at

$$e_0(q) = \frac{b}{2}e_0(q)[J_1(b\xi)]_q + \frac{i}{2}X_{-h}\gamma_1 e_h(q)[J_0(b\xi)]_q. \tag{15}$$

The square brackets indicate a Laplace transform of the function they contain; this transform depends on the argument q. The handbook [18] contains integral no. 6.646.1, which can be transformed as follows:

$$\left[\left(\frac{\xi}{\xi + a}\right)^{n/2} J_n(b[\xi(\xi + a)]^{1/2})\right]_q = \frac{b^n \exp(a_2(q - u))}{u(q + u)^n}, \tag{16}$$

where

$$a_2 = a/2, \quad u = (q^2 + b^2)^{1/2}. \tag{17}$$

Then we substitute (16) at $a = n = 0$ into (15) and make the following calculations, using the designation $W = iX_{-h}\gamma_1/2$:

$$e_0(q) = We_h(q)\left(\frac{[J_0(b\xi)]_q}{1 - (b/2)[J_1(b\xi)]_q}\right) = \frac{We_h(q)}{u - (b^2/2)(u + q)^{-1}}. \tag{18}$$

It can be shown that the denominator in the right-hand side of (18) is equal to $(u + q)/2$ and the inverse function $2/(u + q)$ is the Laplace transform of function $U(b\xi)$, where

$$U(x) = 2\frac{J_1(x)}{x}. \tag{19}$$

After the inverse replacement of variables $\xi \to \xi_\eta - \xi$, we obtain a solution to integral Eq. (13) in the form

$$e_0(\xi_\eta) = \frac{i}{2}X_{-h}\gamma_1\int_0^{\xi_\eta} d\xi U(b[\xi_\eta - \xi])e_h(\xi). \tag{20}$$

Let us consider Eq. (5). In this case, the situation is more difficult, because the argument of the Bessel function depends on the coordinates of point p on the ab line. These coordinates are $z_p = t_0 = \xi_0\cos\theta$ and $x_p = -\xi_0\sin\theta - \eta$. The coordinates of the point on the segment dp' are determined by (8). As a result of simple calculations we easily arrive at

$$s_{op} - s_o = \gamma_1\xi_d,$$
$$s_{hp} - s_h = \gamma_2(\xi_d + a), \quad \xi_d = \xi_\eta - \xi, \tag{21}$$

$$R = J_0(b\sigma_\xi), \quad \frac{\partial R}{\partial s_0} = \frac{b\varsigma_\xi}{2\gamma_1}J_0(b\sigma_\xi),$$
$$a = \varepsilon\eta, \quad \varepsilon = D_1 + D_2, \tag{22}$$

$$\sigma_\xi = (\xi_d[\xi_d + a])^{1/2},$$
$$\varsigma_\xi = \left(\frac{\xi_d + a}{\xi_d}\right)^{1/2}, \quad D_2 = \frac{\gamma_0}{\sin(\theta_B + \theta)}. \tag{23}$$

Taking into account the above-described relations, Eq. (5) can be written as

$$e_h(\eta) = e_h(\xi_\eta) - \frac{b}{2}\int_0^{\xi_\eta} d\xi e_h(\xi)\varsigma_\xi J_1(b\sigma_\xi) - \frac{i}{2}X_h\gamma_2\int_0^{\xi_\eta} d\xi e_0(\xi)J_0(b\sigma_\xi). \tag{24}$$

These integrals are also convolutions of two functions; therefore, it is convenient to use the Laplace transform (however, we have functions of more complex arguments in this case). Let us apply a Laplace transform to the third term in (24) and substitute (18). Taking into account formula (16), we obtain

$$\frac{b}{2}e_h(q)\frac{b\exp(a_2(q-u))}{u(q+u)} = \frac{b}{2}e_h(q)\left[\left(\frac{\xi}{\xi+a}\right)^{1/2} J_1(b[\xi(\xi+a)]^{1/2})\right]_q. \quad (25)$$

Having made a transition from the q space back to the ξ space and added the first term, we obtain the following expression for the sum of the second and the third terms:

$$-\frac{b}{2}\int_0^{\xi_\eta} d\xi e_h(\xi)J_1(b\sigma_\xi)\left[\left(\frac{\xi_d+a}{\xi_d}\right)^{1/2} - \left(\frac{\xi_d}{\xi_d+a}\right)^{1.2}\right]. \quad (26)$$

Performing calculations for the wave function of the reflected beam on the ab line, we obtain a more convenient formula instead of (24):

$$e_h(\eta) = e_h(\xi_\eta) - \frac{1}{4}b^2\varepsilon\eta\int_0^{\xi_\eta} d\xi e_h(\xi) \times U(b([\xi_\eta-\xi][\xi_\eta-\xi+\varepsilon\eta])^{1/2}). \quad (27)$$

This formula expresses the unknown function $e_h(\eta)$ on the ab line in terms of the known function $e_h(\xi)$ on the bd line. This function is known, because the function $E_h(\mathbf{r})$ on this line is simply transferred from the de line in the reflected-beam direction (i.e., its values at points p' and p'' are identical, and the difference can easily be calculated).

The formula for the function $e_0(\eta)$ on the ab line can be obtained similarly to (24) with some evident changes:

$$e_0(\eta) = \frac{b}{2}\int_0^{\xi_\eta} d\xi e_0(\xi)\frac{1}{\varsigma_\xi}J_1(b\sigma_\xi) + \frac{i}{2}X_{-h}\gamma_1\int_0^{\xi_\eta} d\xi e_h(\xi)J_0(b\sigma_\xi). \quad (28)$$

Let us apply a Laplace transform to the first term on the right-hand side, taking into account (25), and substitute expression (18) for $e_0(q)$. As a result, we obtain an expression equal to the second term if $J_0(b\sigma_\xi)$ is replaced by $J_2(b\sigma_\xi)\zeta_\xi^{-2}$. Correspondingly, we arrive at

$$\frac{J_0(b\sigma_\xi)(\xi_d+a) + J_2(b\sigma_\xi)\xi_d}{\xi_d+a} = \frac{U(b\sigma_\xi)\xi_d + J_2(b\sigma_\xi)a}{\xi_d+a}. \quad (29)$$

Here, the relation $J_0 + J_2 = U$ is used. The solution can be written as

$$e_0(\eta) = \frac{i}{2}X_{-h}\gamma_1\int_0^{\xi_\eta} d\xi U_1(\xi_\eta-\xi,\eta)e_h(\xi), \quad (30)$$

where

$$U_1(\xi,\eta) = \frac{\xi U(b[\xi(\xi+\varepsilon\eta)]^{1/2}) + \varepsilon\eta J_0(b[\xi(\xi+\varepsilon\eta)]^{1/2})}{\xi+\varepsilon\eta}. \quad (31)$$

The functions on the bc line can be calculated more easily. In particular, the field $E_h(\mathbf{r})$ on this line is simply transferred from the de line in the reflected-beam direction; in the case of incident plane wave, it is independent of the x coordinate. The field $E_0(\mathbf{r})$ is transferred from the bd line in the transmitted-beam direction. Therefore, the fields at points p_0 and p' are similar. The field $E_0(\mathbf{r})$ on the bd line is calculated from formula (20).

RESULTS AND DISCUSSION

Let us consider the same parameters as in the first part of the study: the photon energy $E = \hbar\omega = 10$ keV, $t_1 = 1$ mm, silicon crystal, reflection 220, and Bragg angle $\theta_B = 18.84°$. Taking into account (4), one can obtain the following expression for the function $e_h(\xi)$ on the bd line:

$$e_h(\xi) = C_h F_h^{-1}(t_1)[F_0^{-1}(\gamma\xi) - F_h^{-1}(\gamma\xi)]. \quad (32)$$

It is convenient to analyze the ratio of the beam intensities over the total thickness t in a crystal with a step with respect to the corresponding ratio for a crystal without a step. To this end, we will consider the ratio $R_h(\eta) = E_h(\eta)/A_h(t)$ on the ab line. Then, taking into account (4), we derive from (27)

$$R_h(\eta) = 1 + g_h(\gamma D_1\eta) - G_h(\eta), \quad (33)$$

where

$$G_h(\eta) = \frac{1}{4}b^2\varepsilon\eta\int_0^{\xi_\eta} d\xi g_h(t_0-\gamma\xi) \times U(b([\xi_\eta-\xi][\xi_\eta-\xi+\varepsilon\eta])^{1/2}), \quad (34)$$

$$g_h(x) = CF_0(x) - F_h(x), \quad C = F_h(t_0)F_0^{-1}(t_0). \quad (35)$$

It is also convenient to make a replacement of variables $\xi = \xi_\eta - \xi_1$ in the integral $G_h(\eta)$ without changing the integration limits. Finally, we arrive at

$$G_h(\eta) = \frac{1}{4}b^2\varepsilon\eta\int_0^{\xi_\eta} d\xi_1 \times g_h(\gamma D_1\eta + \gamma\xi_1)U(b(\xi_1[\xi_1+\varepsilon\eta])^{1/2}). \quad (36)$$

Note that the second and third terms in (33) are zero at $\eta = \eta_m = t_0/\gamma D_1$, and the ratio is equal to unity (i.e., the solution is continuous at the Borrmann triangle boundary). At $\eta = 0$, the parameter $R_h(0) = F_h(t_0)/F_0(t_0)$, and the relative intensity depends only slightly on the step height; however, the real intensity is independent of the step height and equals to the field intensity at the thickness t_1.

Thus, the formula for the relative intensity contains three terms; the second and the third are complex. Therefore, if the absolute values of all three terms are close, they in sum can formally increase the intensity by a factor of 9. As was shown in [1], a numerical calculation leads to an increase in the intensity peaks by a factor of more than 7. The mechanism of this increase can be understood by analyzing formula (33).

Taking into account (4), one can derive from formula (30) a formula for $R_0(\eta) = E_0(\eta)/A_0(t)$ ratio on the *ab* line:

$$R_0(\eta) = 1 - G_{01}(\eta), \quad (37)$$

where

$$G_{01}(\eta) = \frac{i}{2} X_{-h}\gamma_1 \int_0^{\xi_\eta} d\xi_1 g_h(\gamma D_1\eta + \gamma\xi_1) U_1(\xi_1, \eta). \quad (38)$$

Formula (37) contains only two terms; i.e., the intensity maximum can formally increase by a factor of 4.

Let us consider the ratio $R_0(\eta) = E_0(\eta)/A_0(t)$ on the *bd* line. In this case, the coordinate η is counted from the point *b* to the point *d*, and $\xi_\eta = \xi_0 - \eta D_2$. The point p' corresponds to the point p_0 in Fig. 1a. Having made the same transformations as before, we obtain

$$R_0(\eta) = F_0^{-1}(\gamma D_2\eta)[F_h(\gamma D_2\eta) - G_{02}(\eta)], \quad (39)$$

where

$$G_{02}(\eta) = \frac{i}{2} X_{-h}\gamma_1 \int_0^{\xi_\eta} d\xi_1 g_h(\gamma D_2\eta + \gamma\xi_1) U(b\xi_1). \quad (40)$$

Formula (39) was derived taking into account that field strength E_0 at the points η on the segment *bc* and ξ_η on the segment *bd* is the same and that $C_h = -C_0$. At $\eta = 0$, formula (39) yields the same value as (37), and at $\eta = \eta_m = t_0/\gamma D_2$ the expression can be written as $F_h(t_0)/F_0(t_0)$ (i.e., it slightly exceeds unity, because a real field is not absorbed at height t_0 and the denominator in the ratio corresponds to the thickness *t*).

Figure 1b shows three types of step inclination, which can be characterized by different values of parameter $R = \tan\theta/\tan\theta_B$ when the angle θ is counted as shown in Fig. 1a. Figure 2 presents the distributions of the relative intensity $I/I_0 = |R_{0,h}|^2$ of the transmitted (*T*) and reflected (*R*) beams on the Borrmann triangle base *ac*, calculated from formulas (33), (37), and (39) at $t_0 = 0.2$ mm and $R = 0.5$, 0, and –0.5, respectively. The calculation results obtained by the numerical method [1] for the same parameters coincide with the data of this study. It is of interest that the calculation result of [1] for $L = 2$ m barely differs from the result shown in Fig. 2a. The reason is that a thick crystal forms a divergent spherical wave at a small distance from a point radiation source, which almost coincides in the step region with a plane wave.

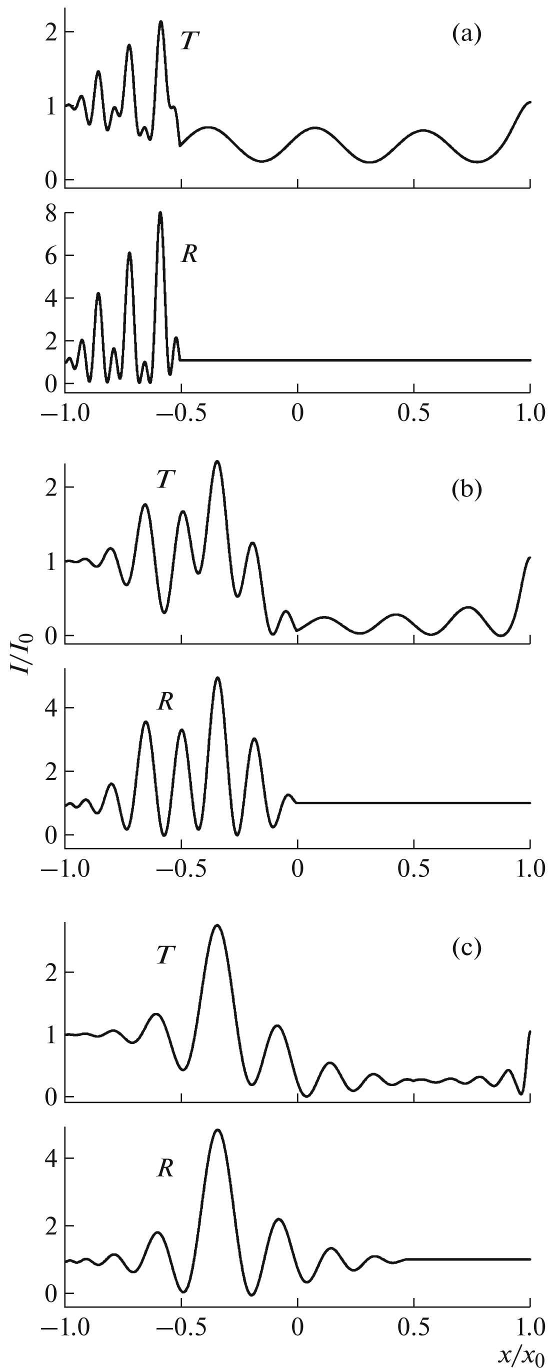

Fig. 2. Dependences of the relative intensity of the (*T*) transmitted and (*R*) reflected beams on the element of exit surface coinciding with the Borrmann triangle base (*ac* line in Fig. 1a) at $x_0 = 68.2$ μm and $R =$ (a) 0.5, (b) 0, and (c) –0.5.

The calculations showed that the most interesting results are obtained at a positive, close-to-unity value of parameter *R*. In this case, the reflected-beam intensity oscillates with a short period and has the largest values (close to 9) in maxima. However, this does not occur always but depends periodically on the step height.

The relative reflected-beam intensity exceeds that of the incident beam at $|R| < 1$. At $|R| > 1$, formulas (33), (37), and (39) are not applicable, and the calculation must be performed in a different way. Note that there is some correlation between the intensity maxima and minima of the transmitted and reflected beams (they occur simultaneously). That is why these oscillations differ from the extinction oscillations of plane wave intensity in dependence on the crystal thickness, when the transmitted-beam intensity is transferred into the reflected-beam intensity and vice versa.

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