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DIFFRACTION AND SCATTERING OF IONIZING RADIATION

Trajectory Method in the Theory of Laue Diffraction of X-rays in Crystals: I. General Formulas and Accuracy Estimation

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Abstract—The most general and successive formulation of the trajectory method for solving the Takagi equations in the description of diffraction of a spatially inhomogeneous X-ray wave in ideal and deformed crystals is presented. The trajectories are obtained by variation in the common phase of the transmitted and diffracted waves similarly to classical mechanics. An algorithm of numerical calculation using the trajectory method has been developed and the results of the calculations are reported for the case of diffraction of a spherical wave in an ideal crystal. It is shown that the trajectory method provides high numerical accuracy in description of pendellosung fringes everywhere except for peculiar points, where trajectories approach very close to each other.

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INTRODUCTION

The diffraction of a spatially inhomogeneous X-ray wave in ideal and deformed crystals is described with high accuracy by the Takagi equations [1]. In the case of an ideal crystal, the exact solution can be obtained in an integral form using the response function, i.e., the analytical solution of the equations for a point source on the surface (for example, [2]) or by double Fourier transformation using an analytical solution for a plane wave. In a crystal with a slowly varying strain, an approximate solution can be obtained by integration over trajectories using the classical mechanics apparatus. This method was proposed for the first time in [3–5] for the Maxwell equations and then extended to the Takagi equations [6].

Despite certain limitations, the trajectory method is extremely useful since it gives a simple and descriptive pattern of radiation propagation in the form of set of rays. At the same time, being used in numerical simulation, it allows one to significantly reduce the calculation time in comparison with the direct solution of the Takagi equations. Initially, the trajectory method was applied to study pendellosung fringes in elastically bent crystals, but after finding the response function for a crystal with a constant strain gradient [6], it was undeservedly forgotten.

Recently, X-ray diffraction in crystals deformed by long-wavelength ultrasound was investigated [7, 8]. In this case, the strain induced cannot be approximated by a constant gradient. The use of the trajectory method for description of the physical phenomena observed in these experiments is of great interest.

In this paper, we present the most general and successive formulation of the trajectory method for solving the Takagi equations. Note that this method was described in [6] only for a symmetric case, insufficiently correctly, and with a large number of errors. In addition, the algorithm of the program for using this method in numerical calculations is described here in detail. The results of the calculation by this program in the case of diffraction of a spherical wave are compared with the results of the calculation based on double Fourier transformation. This comparison makes it possible to quantitatively estimate the accuracy of the trajectory method during numerical simulation of an experiment.

GENERAL FORMULAS

Let coherent monochromatic X-ray radiation with a spatially inhomogeneous electric field $E_{0i}(\mathbf{r})\exp(i\mathbf{K}_0\mathbf{r})$ be incident on a crystal and the field amplitude $E_{0i}(\mathbf{r})$ be almost constant at distances of about the radiation wavelength. The Laue diffraction conditions are satisfied in the crystal. The field in the crystal can be written in the form

$$E(x, z) = E_0(x, z)\exp(i\mathbf{K}_0\mathbf{r}) + E_h(x, z)\exp(i\mathbf{K}_h\mathbf{r}),$$
$$\mathbf{K}_h = \mathbf{K}_0 + \mathbf{h}, \quad (1)$$

where $\mathbf{h}$ is the reciprocal lattice vector of the crystal in the absence of strain and x and z are the coordinates in the scattering plane parallel and perpendicular to the crystal surface, respectively; the x axis is directed toward the incident beam. The amplitudes E_0 and E_h are

also almost constant at distances of about the radiation wavelength. Expression (1) was written for amplitudes in the case of one of two possible polarization states, specifically, with polarizations directed perpendicularly to the scattering plane (σ) and lying in the scattering plane (π).

According to [2], the equations for the amplitudes E_0 and E_h can be obtained by substituting expression (1) into the Maxwell equation and neglecting the second derivatives of the amplitudes. As a result, we have

$$\begin{aligned} i\frac{\partial E_0}{\partial s_0} + c_0 E_0 + c_{\bar{h}} F^* E_h &= 0, \\ i\frac{\partial E_h}{\partial s_h} + (c_0 - a_0) E_h + c_h F E_0 &= 0. \end{aligned} \tag{2}$$

Here, $c_0 = K\chi_0/2$; $c_m = KC\chi_m/2$, $m = h$ or $\bar{h}$; χ_0, χ_h, and $\chi_{\bar{h}}$ are the Fourier components of the crystal polarizability on the reciprocal lattice vectors 0, $\mathbf{h}$, and $-\mathbf{h}$, respectively; $K = |\mathbf{K}_0|$; $K_h = |\mathbf{K}_h|$; $a_0 = (K_h^2 - K^2)/2K$; $F = \exp(-i\mathbf{h}[\mathbf{u}(\mathbf{r}) + \mathbf{u}_0])$; and the function $\mathbf{u}(\mathbf{r})$ describes the field of strain-induced atomic displacements. The value of F^* is complex conjugate to F. Differentiation is performed over coordinates along the directions of the incident (s_0) and reflected (s_h) beams. The polarization factor $C = 1$ and $\cos(2\theta_B)$ for the σ and π polarizations, respectively, and θ_B is the Bragg angle.

Generally, the complex scattering parameters have the following form: $c_h = -c + i\nu_h = -c(1 - iw_h)$ and $c_{\bar{h}} = -c + i\nu_h^* = -c(1 - iw_h^*)$; $|\,|w_h| \ll 1$. Here, $c = KC|\chi_{rh}|/2$ is a real number, and the phase of the complex parameter χ_{rh} in the form of the factor $\exp(-i\mathbf{hu}_0)$ is explicitly taken into account in the equations in terms of the phase factor F. Accordingly, $\nu_h = \chi_{ih}\exp(i\mathbf{hu}_0)$. The subscripts r and i indicate the contributions of elastic and inelastic processes to the polarizability. Taking explicitly into account the smallness of w_h, we will use the linear approximation in this parameter. Then, $c_h c_{\bar{h}} = c(1 - 2ig)$, where $g = \mathrm{Re}(w_h)$. In a centrosymmetric crystal, $\mathbf{u}_0$ corresponds to the center of a unit cell, and the parameter w_h is a real number.

Oblique coordinates s_0 and s_h are related to the Cartesian coordinates x and z as follows: $x = s_0\sin\theta_0 - s_h\sin\theta_h$ and $z = s_0\cos\theta_0 + s_h\cos\theta_h$, where θ_0 and θ_h are, respectively, the angles made by the vectors of the incident and diffracted waves with the internal normal to the crystal surface. It is obvious that $\theta_0 + \theta_h = 2\theta_B$. The inverse relations can easily be obtained by solving the system of equations.

The Takagi equations (2) can be reduced to a simpler form by the substitution $E_0 = E_0' B$ and $E_h = E_h' BF$, where $B = \exp(ic_0[s_0 + s_h])$:

$$i\frac{\partial E_0'}{\partial s_0} + c_{\bar{h}} E_h' = 0, \quad i\frac{\partial E_h'}{\partial s_h} - aE_h' + c_h E_0' = 0, \tag{3}$$

where the coordinate-dependent parameter $a = a_0 - \partial(\mathbf{hu}(\mathbf{r}))/\partial s_h$ describes the local deviation from the Bragg condition with allowance for the lattice strain.

It is known that, in an ideal crystal, for each polarization state, there are two combinations of waves differing in absorption and having the same phase for the transmitted and reflected waves. In this study, we consider only slowly varying deformation, for which the relative change in strain on the extinction length is small. In this case, two combinations of waves exist also in the deformed crystal and it is reasonable to search for a solution with the same phase; i.e., $E_{0,h}' = E_{0,h}'' \exp(i\Phi)$, where the amplitudes $E_{0,h}''$ and the phase Φ are real values in an nonabsorbing crystal. Substituting such a solution into (3), we obtain

$$\begin{aligned} -\frac{\partial \Phi}{\partial s_0} E_0'' + c_{\bar{h}} E_h'' + i\frac{\partial E_0''}{\partial s_0} &= 0, \\ -\frac{\partial \Phi}{\partial s_h} E_h'' - aE_h'' + c_h E_0'' + i\frac{\partial E_h''}{\partial s_h} &= 0. \end{aligned} \tag{4}$$

To solve this system, it is necessary to equate the real and imaginary parts to zero independently. Selecting the real part, we obtain the system of linear equations with variable coefficients:

$$\begin{aligned} -\frac{\partial \Phi}{\partial s_0} E_0'' + c_{\bar{h}} E_h'' &= 0, \\ -\frac{\partial \Phi}{\partial s_h} E_h'' - aE_h'' + c_h E_0'' &= 0. \end{aligned} \tag{5}$$

A necessary condition for the existence of a nonzero solution for this system is the equality of its determinant to zero at each point. This condition yields an equation directly for the phase. Let us write this equation, while passing to new variables along and across the beam direction: $X = s_0 - s_h$ and $Z = s_0 + s_h$. After a slight transformation, the equation can be written as

$$\left(\frac{\partial \Phi}{\partial Z} + \frac{a}{2}\right)^2 - \left(\frac{\partial \Phi}{\partial X} - \frac{a}{2}\right)^2 = c_h c_{\bar{h}}. \tag{6}$$

With allowance for absorption, the right-hand side of this equation is complex; therefore, the phase $\Phi = \Phi_r + \Phi_i$ is also complex with a relatively small imaginary part. We will solve the equation for the real part of the phase by the variational method, using the apparatus of classical mechanics [9]. Considering Φ_r as an action function (eikonal) and the Z coordinate as an analogue of time, we will introduce the Hamiltonian

H and the generalized momentum P and determine the analogues for the imaginary part of the phase:

$$H = -\frac{\partial \Phi_r}{\partial Z}, \quad P = \frac{\partial \Phi_r}{\partial X}, \quad \Gamma = -\frac{\partial \Phi_i}{\partial Z}, \quad Q = \frac{\partial \Phi_i}{\partial X}. \quad (7)$$

In the approximation linear in the small parameter g, we find from (6) that

$$\begin{gathered}\left(H - \frac{a}{2}\right)^2 - \left(P - \frac{a}{2}\right)^2 = c^2, \\ \left(H - \frac{a}{2}\right)\Gamma - \left(P - \frac{a}{2}\right)Q = -gc^2.\end{gathered} \quad (8)$$

The first equation in (8) determines the dependence $H(P)$. The trajectory $X(Z)$ is obtained by variation in the action function. It is known that the velocity on a trajectory is

$$V = \frac{dX}{dZ} = \frac{\partial H}{\partial P} = \pm\frac{y}{(1 + y^2)^{1/2}}, \quad y = \frac{P - a/2}{c}. \quad (9)$$

To calculate the real part of the phase in the form of an integral over Z, it is necessary to introduce the Lagrangian

$$L = \frac{d\Phi_r}{dZ} = \frac{\partial \Phi_r}{\partial Z} + V\frac{\partial \Phi_r}{\partial X} = VP - H. \quad (10)$$

The Lagrangian is a function of the coordinate and velocity. Expressing P and H in terms of V with the use of (9), we obtain

$$\begin{gathered}\frac{P - a/2}{c} = y = \pm\frac{V}{(1 - V^2)^{1/2}}, \\ \frac{H - a/2}{c} = \pm(1 + y^2)^{1/2} = \pm\frac{1}{(1 - V^2)^{1/2}}.\end{gathered} \quad (11)$$

Substitution of (11) into (10) gives

$$L = \mp c(1 - V^2)^{1/2} - \frac{a}{2}(1 - V). \quad (12)$$

The Lagrange equation, which determines the trajectory, is conventionally written as

$$\frac{dP}{dZ} = \frac{\partial L}{\partial X} = -\frac{1}{2}(1 - V)\frac{\partial a}{\partial X}. \quad (13)$$

It is convenient to write this equation in terms of the dimensionless variable y and with allowance for (9). As a result, we obtain

$$\begin{gathered}\frac{dy}{dZ} = -\frac{1}{2c}\left(\frac{\partial}{\partial Z} + \frac{\partial}{\partial X}\right)a \\ = -\frac{1}{2c}\frac{\partial a}{\partial s_0} = \frac{1}{2c}\frac{\partial^2}{\partial s_0 \partial s_h}(\mathbf{hu}(\mathbf{r})).\end{gathered} \quad (14)$$

Thus, the Z coordinate is independent, Eq. (14) determines the variable y as a function of Z, and the velocity V on the trajectory is expressed in terms of y with the use of (9). Two signs determine two trajectories for two possible solutions. The real part of the phase is calculated as an integral of Lagrangian (10) over Z. The imaginary part of the phase must be calculated on the same trajectory, but it is necessary to know the complete derivative with respect to Z. It turns out that the second equation in (8) gives the necessary combination:

$$\frac{d\Phi_i}{dZ} = VQ - \Gamma = \frac{gc^2}{H - a/2} = \pm gc(1 - V^2)^{1/2}. \quad (15)$$

We can disregard absorption in calculation of the amplitudes $E''_{0,h}$. In this case, it follows from the first equation of system (5) that $E''_h/E''_0 = R = (H - P)/c$. Thus, it is sufficient to obtain the equation only for $E''_0 = \sigma(\mathbf{r})$. To this end, we will use the imaginary parts of the system of equations (4). Multiplying the first and second equations by E''_0 and E''_h, respectively, and summing them, we obtain the desired equation in the form of the law of conservation of energy flux: $\operatorname{div}\mathbf{S} = 0$, where $\mathbf{S} = \mathbf{s}_0(E''_0)^2 + \mathbf{s}_h(E''_h)^2$, $\mathbf{s}_0 = \mathbf{K}_0/K$, and $\mathbf{s}_h = \mathbf{K}_h/K_h$; i.e.,

$$\frac{\partial}{\partial s_0}(E''_0)^2 + \frac{\partial}{\partial s_h}(E''_h)^2 = 0. \quad (16)$$

Passing to the X and Z coordinates and using the expression for the ratio of the amplitudes in the form of a velocity function, one can show that this equation on a trajectory is reduced to

$$\frac{d}{dZ}\left(\frac{\sigma}{(1 + V)^{1/2}}\right) = 0. \quad (17)$$

Formulas (12), (14), (15), and (17) make it possible to calculate the complex phase and real wave amplitudes on a trajectory by simple integration over Z with allowance for the dependence $X(Z)$. It can be shown that the direction of the energy flux at each point coincides with the direction of the tangent to the trajectory.

ALGORITHM OF NUMERICAL CALCULATION

Propagation of X rays in a homogeneous medium (including air) can be described by the paraxial approximation, in which the amplitude variation length in the direction of the wave vector (optical axis) exceeds the variation length in the direction perpendicular to the optical axis by more than several thousands. Therefore, it is the slow change (transport) in the transverse dependence of the wave field along the optical axis that is of interest. This problem can be solved with a sufficient accuracy using Kirchhoff integrals in the paraxial approximation. For this reason, it is desirable to represent the solution to the problem of radiation diffraction

in a crystal as the transport of the transverse dependence of a wave.

In the general case of asymmetric diffraction, the rectangular coordinate systems (X, Z) and (x, z) are rotated with respect to each other by the angle $(\theta_0 - \theta_B)$. In the further description of the algorithm, we will consider only the Laue symmetric diffraction. In this case, the above-mentioned angle is zero, $x = X\sin\theta_B$, $z = Z\cos\theta_B$, and $s_0 + s_h = z/\cos\theta_B$. Let us assume that the transverse structure of radiation in front of the crystal as a function of the coordinates x_b and y_b is known. The coordinate y_b is an external parameter and will not be explicitly indicated below. Let us project the field on the input crystal surface, while taking into account that $x_b = x\cos\theta_B$, and represent the complex function $E_{0i}(x)$ in the form $E_{0i} = E''_{0i}\exp(i\Phi_0)$, where E''_{0i} and Φ_0 are real values and Φ_0 is a continuous function of the X coordinate. Generally, the input radiation is set on a grid with a very small constant step because fast Fourier transformation [10] is used to calculate the input radiation; therefore, it is fairly easy to eliminate 2π jumps in phase.

Choosing a larger grid of X_0 points with a constant step d on the input crystal surface ($Z = 0$) as the initial points of the system of trajectories, we obtain the initial value of the deviation from the Bragg condition by the formula

$$y_0 = \frac{1}{c}\left(\frac{\partial\Phi_0}{\partial X}\right)_{X_0} - \frac{a(X_0, 0)}{2c}. \tag{18}$$

Let h denote the constant step of variation in the Z coordinate. The next value of y at $Z = h$ will be found from Eq. (14):

$$y_1 = y_0 - -\frac{h}{2c}\left(\frac{\partial}{\partial Z} + \frac{\partial}{\partial X}\right)a(X_0, 0). \tag{19}$$

At each value of y, we have, according to (9), two velocities $V^{(k)}(y)$, $k = 1, 2$, on two trajectories for two fields, which differ in absorption. The points on the trajectory can be calculated by the trapezoid method, specifically

$$Z_1 = Z_0 + h, \quad X_1^{(k)} = X_0^{(k)} + \frac{h}{2}(V_0^{(k)} + V_1^{(k)}). \tag{20}$$

The next trajectory points are obtained by iteration of formulas (19) and (20) after replacement of the subscripts 0 and 1 with m and $m + 1$, respectively.

Concerning the phase, it can be found by calculating the integrals of functions (12) and (15) over the trajectory by the trapezoid method. In this case, the result is reduced to the sum over points on the Z axis at known dependences of X and V on Z. To calculate the amplitudes, it is necessary to use in the initial stage the boundary conditions on the input surface. We have two values of $\sigma_i^{(k)}$ for the amplitude of the transmitted wave and two known values of $R_i^{(k)}$ for the amplitude ratio. To calculate $\sigma_i^{(k)}$, we have the equations

$$\begin{gathered} E''_{0i} = \sigma_i^{(1)} + \sigma_i^{(2)}, \quad 0 = \sigma_i^{(1)}R_i^{(1)} + \sigma_i^{(2)}R_i^{(2)}, \\ R_i^{(k)} = -y_0 \pm (1 + y_0^2)^{1/2}. \end{gathered} \tag{21}$$

Solving the system of equations and expressing y in terms of V, one can write the answer as

$$\sigma_i^{(k)} = \frac{1}{2}E''_{0i}(1 + V_0^{(k)}). \tag{22}$$

Let the crystal thickness be $t = hM$. On the output crystal surface, according to (17), we have

$$\begin{gathered} \sigma_o^{(k)} = \sigma_i^{(k)}\left(\frac{1 + V_M^{(k)}}{1 + V_0^{(k)}}\right)^{1/2}, \\ R_o^{(k)} = \pm(1 - V_M^{(k)})^{1/2}(1 + V_M^{(k)})^{-1/2}. \end{gathered} \tag{23}$$

Substituting (22) into (23) and performing calculations, we obtain

$$\begin{gathered} E''_{0k} = \frac{1}{2}E''_{0i}(1 + V_0^{(k)})^{1/2}(1 + V_M^{(k)})^{1/2}, \\ E''_{hk} = \pm\frac{1}{2}E''_{0i}(1 + V_0^{(k)})^{1/2}(1 - V_M^{(k)})^{1/2}. \end{gathered} \tag{24}$$

Formulas (18)–(24) make it possible to calculate all quantities on each trajectory. However, this is insufficient for calculating the local intensity. The density of trajectories at each point on the output surface is important also. Let n denote the trajectory number. Then, it is necessary to multiply the amplitudes of the nth trajectory at the output by the factor

$$D^{(k,n)} = \left(\frac{1}{2d}[X_M^{(k,n+1)} - X_M^{(k,n-1)}]\right)^{-1/2}. \tag{25}$$

If trajectories cross each other, factor (25) becomes imaginary. In this case, the amplitudes are multiplied by the absolute value of this factor and the phase Φ_r should be increased by $\pi/2$. The refined amplitude and phase will be denoted from above by ~.

The last operation is interpolation of the amplitudes and phases for the two combinations of waves to a standard point grid perpendicularly to the beam direction, i.e., with allowance for the relations $x_b = x\cos\theta_B = X\sin(2\theta_B)/2$. After the interpolation, the trajectory number is replaced with the x_b coordinate. However, we should also take into account that the trajectories may rotate and multiply pass through the same point. Therefore, during summation of complex amplitudes into a single point, it is necessary to scan all trajectories and sum each pass. The number of each pass will be denoted by index l.

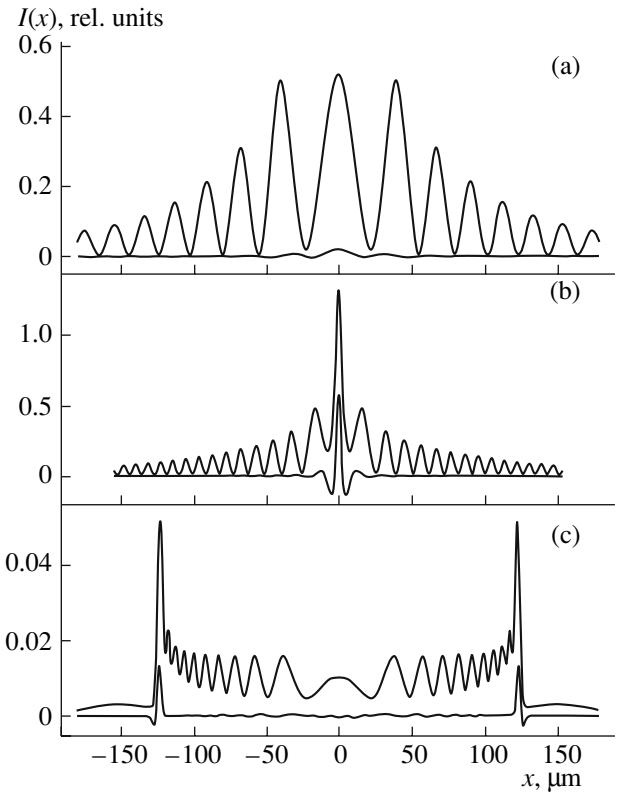

Fig. 1. Pendellosung fringes in the case of diffraction of a spherical X-ray wave in an ideal crystal. The upper curves of relative intensity are calculated by the trajectory method and the lower curves are the differences between the upper curves and the curves calculated by the exact method of double Fourier transformation; silicon crystal; 220 reflection; σ polarization; (a) the source-to-crystal distance R = (a) 10, (b) 10, and (c) 1 m; the crystal thickness t = (a) 100, (b) 250, and (c) 800 μm. The x axis is perpendicular to the beam direction.

As a result, the formulas for the complex amplitude at the point x_b at the crystal output can be written as

$$E_0 = \sum_{k=1,2}\sum_{l}\tilde{E}''_{0k}\exp(\Psi_k),$$

$$E_h = F\sum_{k=1,2}\sum_{l}\tilde{E}''_{hk}\exp(\Psi_k), \tag{26}$$

$$\Psi_k = -\chi_{i0}T - \Phi_{ik} + i[\chi_{r0}T + \tilde{\Phi}_{rk}], \quad T = \frac{Kt}{2\cos\theta_B}.$$

Note that the phase factor F can play a significant role in the subsequent transmission of a reflected wave along the optical axis behind the crystal.

The above-considered algorithm of calculation of the wave field in the case of Laue X-ray diffraction was implemented as a program written with the programming languages Java [11] and ACL [12].

DIFFRACTION OF A SPHERICAL WAVE IN AN IDEAL CRYSTAL

Here, the results of program testing by the example of spherical wave diffraction in an ideal crystal are presented. This case is convenient because the result can be obtained both by the approximate trajectory method and by the exact method based on double Fourier transformation with the use of the analytical formula for the reflected-wave amplitude.

Since strain is absent in the crystal, all trajectories are straight lines and the angle of trajectory inclination is determined by formulas (9) and (18). The phase of a spherical wave on the crystal surface, expressed in terms of the X coordinate, is $\Phi_0 = (K/8R)\sin^2(2\theta_B)X^2$, where R is the distance between the point source and crystal and the amplitude is constant and arbitrarily equal to unity. Calculating the derivative, we obtain the deviation from the Bragg condition in the form $y_0 = (K/4cr)\sin^2(2\theta_B)X$. In the center of the beam, $|y_0| \ll 1$ and the angle of inclination $(dX/dZ) \sim \pm y_0$; i.e., it depends linearly on X. At plus and minus, the trajectories diverge and converge, respectively. At a certain crystal thickness $t = t_f$, all trajectories cross each other at one point, where

$$t_f = \frac{|\chi_{rh}|C}{\sin\theta_B\sin(2\theta_B)}R. \tag{27}$$

Formula (27) was obtained for the first time in [13]. Accordingly, for this zone of the wave field at $t < t_f$, the order of trajectories is retained; at $t > t_f$ in the central part, the order becomes inverted. Far from the beam center, the trajectories are almost parallel to the direction of the transmitted and reflected waves. Therefore, the trajectories crowd at $x_b \approx \pm(t - t_f)\sin\theta_B$ to form caustics. Obviously, both in the focal and caustic regions, the trajectory method cannot be used, whereas double Fourier transformation gives exact results in this case.

The figure shows the results of calculation for a silicon crystal, 220 reflection, σ polarization, and the photon energy E = 17.48 keV (MoK_α line). In this case, θ_B = 10.643°, and for R = 10 m, the crystal focuses at the thickness t_f = 286.1 μm. The figure consists of three fragments, with two curves in each. The upper curve is the relative intensity of the reflected beam directly behind the crystal calculated by the trajectory method described above. The lower curve is the difference between the upper curve and the exact curve calculated by double Fourier transformation. In the calculation by the trajectory method, the initial wave field was determined on a grid of 16384 points with a 0.25-μm step. In the same region, 1024 trajectories were used. For the exact curves, the point grid step was the same, but the number of points and the model region were larger by a factor of 4. Such an increase is necessary to obtain the required accuracy.

In Fig. 1a, the distance R = 10 m, the crystal thickness t = 100 μm, and the detector resolution is 2 μm (the

curve is convoluted with a Gaussian having a half-width of 2 μm). It can be seen that the trajectory method makes it possible to obtain the pendellosung fringes with very high accuracy. The difference from the exact solution is maximum at the center and does not exceed 3%.

In Fig. 1b, all parameters are the same except for the crystal thickness. Here, $t = 250$ μm, i.e., is close to the focusing thickness. In this case, the trajectory method overestimates the focal distance in comparison with the exact solution by a factor of 1.6. However, this overestimation depends on the detector resolution. The integrated intensities coincide; therefore, the difference decreases at a poorer resolution. Far from the focal point, the pendellosung fringes are obtained with high accuracy.

In Fig. 1c, the distance $R = 1$ m, the crystal thickness $t = 800$ μm, and the detector resolution is 3 μm. In this case, the crystal thickness greatly exceeds the focusing thickness and the relative reflection intensity is low. Pendellosung fringes are very exactly described by the trajectory method, while in the region of caustics both the local and integrated intensities are overestimated. It is of interest that the increase in the number of trajectories makes it possible to reduce the difference of the integrated intensities to some minimum but not to zero. The specificity of this case is that the trajectories are rotated in the caustic region and factor (25) insufficiently correctly describes the intensity.

Thus, the results of the calculations performed here showed that the trajectory method makes it possible to describe the pendellosung fringes with high accuracy everywhere except for peculiar points, where trajectories approach each other at a very small distance. This fact indicates that the trajectory method gives not only a correct qualitative but also an acceptable quantitative pattern of the intensity distribution.

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