Dynamic scattering of x-rays by dislocations

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The geometric diffraction optics of x-rays is considered. The trajectories of rays scattered by an elastic dislocation field are found by employing an analogy between the equations for ray trajectories and equations describing one-dimensional motion of a relativistic particle in an external field. Expressions for the eikonal and amplitudes of a wave field in a crystal are derived in the general case of dynamic scattering of x-rays by a straight dislocation. Scattering by an edge dislocation under conditions of anomalous transmission of x-rays (the Borrmann effect) is analyzed in detail.

1. INTRODUCTION

It is known that the wave field of x-rays in a crystal, under conditions of the dynamic problem, is very sensitive to static deviations of the crystal lattice from the ideal. This is the basis of various x-ray diffraction methods of investigating the internal structure of real crystals. Scattering of x-rays by dislocations in a crystal is furthermore of interest because a suitable choice of the dislocation distribution makes it possible, in principle, to form a wave field with prescribed properties[1]. In particular, focusing of x-rays can take place if the dislocation structure of the crystal is suitably chosen.

The general theory of x-ray scattering in crystals with defects is developed in[2-6]. The principal mechanisms of dynamic scattering of x-rays by dislocations are classified in[2]. An integral form of the theory has been developed in[3,4]. Integral equations equivalent to the modified differential equations of Takagi make it possible to treat by a unified approach both weakly distorted and strongly distorted regions of the crystal[4].

A general theory of diffraction geometric optics of x-rays has been developed in[5,6]. The role of the characteristic wavelength is taken here by the extinction length $\Lambda = \lambda C^{-1}(\chi_{-1}\chi_1)^{-1/2}$ (λ is the x-ray wavelength, C is the polarization factor, and χ_{-1} and χ_1 are the Fourier components of the polarizability of the crystal, corresponding to diffraction with a reflection vector $\mathbf{K}_1$; for x-rays $|\chi_{-1,1}| \sim 10^{-6} - 10^{-5}$), and the role of the inhomogeneities of the medium is assumed by the local deviation $\alpha(x)$ from the Bragg condition.

In the present article we consider, within the framework of geometrical optics, the scattering of x-rays by an elastic dislocation field. In Sec. 2 we present briefly the derivation of the fundamental equations of two-ray geometric optics in an absorbing crystal. A system of differential equations along the x-ray trajectory is given for the eikonal and for the amplitudes of the transmitted and diffracted waves.

Using the analogy between the equation for the ray trajectories and the equation describing one-dimensional motion $x(z)$ of a relativistic particle in an alternating external field $\alpha(x)$, we obtain in Sec. 3 the trajectories of rays scattered by an elastic dislocation field. It is shown that the degree of "relativism" for particles moving along the trajectories is given by $\dot{x}^2 \sim (l_{\text{eff}}/\Lambda)^{-2}$, where l_{eff} is the characteristic length over which the function $\alpha(x)$ varies, while for the trajectories whose minimum distance to the dislocation core exceeds the extinction length we have $\dot{x}^2 \ll 1$. Expressions are obtained for the eikonal and for the wave-field amplitudes in the general case of scattering by a straight-line dislocation. In Sec. 4 we consider the scattering of x-rays by an edge dislocation under conditions of anomalous transmission (the Borrmann effect[7,8]) for strongly absorbing crystals, when the distance of the dislocation from the two surfaces of a plane-parallel crystal is much larger than the length of the photoelectric absorption μ_0^{-1}. In this case there propagates in the crystal a Borrmann wave field of weakly absorbed x-rays interacting with dislocations. It is shown that a shadow is produced behind the dislocation, and that the intensity of the wave field varies like $\exp(-g\mu_0\Lambda^2/|x_2|)$, where x_2 is the longitudinal distance from the center of the shadow (along the reflection vector $\mathbf{K}_1$), g is a numerical coefficient that depends on the "longitudinal dislocation power" (K_{1b}), and b is the Burgers vector of the dislocation.

2. FUNDAMENTAL EQUATIONS OF X-RAY GEOMETRIC OPTICS

If the orientation of the crystal is close to the Bragg position with a reflection vector $\mathbf{K}_1$, a coherent superposition of transmitted and diffracted waves propagates in the crystal. To describe the x-ray wave field in the crystal, one can use Maxwell's equations in the quasiclassical approximation[3,5]:

$$\begin{pmatrix} 2i\mathcal{D}_+ + \chi_0 & \chi_{-1}C\exp\{i\mathbf{K}_1\mathbf{u}(\mathbf{x})\} \\ \chi_1 C\exp\{-i\mathbf{K}_1\mathbf{u}(\mathbf{x})\} & 2i\mathcal{D}_- + \chi_0 \end{pmatrix}\begin{pmatrix} E_0 \\ E_1 \end{pmatrix} = 0. \quad (2.1)^*$$

Here $\mathcal{D}_\pm = (\partial/\partial z \pm \partial/\partial x)$, E_0 and E_1 are the amplitudes of the transmitted and diffracted waves, x and z are the dimensionless coordinates in the x-ray scattering plane (xOz), χ_0 is the average polarizability of the crystal, and $\mathbf{u}(\mathbf{x})$ is the displacement field in the distorted crystal. Details concerning the notation can be found in[5,6].

The substitution $E_0 \to E_0\exp[i\chi_0 z/2]$ and $E_1 \to E_1\exp[i\chi_0 z/2 - i\mathbf{K}_1\cdot\mathbf{u}(\mathbf{x})]$ transforms (2.1) into

$$\begin{pmatrix} i\mathcal{D}_+ & {}^1/_2\chi_{-1}C \\ {}^1/_2\chi_1 C & i\mathcal{D}_- - 2\alpha(\mathbf{x}) \end{pmatrix}\begin{pmatrix} E_0 \\ E_1 \end{pmatrix} = 0. \quad (2.2)$$

The function $\alpha(x)$ of local deviation from the Bragg condition is determined by the displacements of the reflecting planes, and is given by

$$\alpha(\mathbf{x}) = {}^1/_2\mathcal{D}_-(K_1 u_x(\mathbf{x})) \quad (2.3)$$

The substitution used to go from (2.1) to (2.2) does not affect the boundary conditions at the entrance surface of the crystal $z = z_1$ if the amplitudes E_0 and E_1, in the case of a plane wave incident on the crystal, are of the form

$$E_0(x, z_1) = 1, \quad E_1(x, z_1) = 0. \tag{2.4}$$

The problem (2.2)–(2.4) of x-ray propagation in crystals with defects is analogous to the problem of the passage of light through inhomogeneous media. Assuming that the characteristic length l_{eff} of variation of the function $\alpha(x)$ exceeds the extinction length Λ, we can construct the wave field in the crystal by the method of geometrical optics. Accordingly, we separate in the amplitudes E_0 and E_1 the eikonal $S(x)$

$$\hat{E}(x) \equiv \begin{pmatrix} E_0(x) \\ E_1(x) \end{pmatrix} = e^{iS(x)} \sum_{n=0}^{\infty} \hat{E}^{(n)}(x). \tag{2.5}$$

Substitution of (2.5) in (2.2) leads to an infinite system of coupled equations for the eikonal $S(x)$ and the amplitudes $E^{(n)}(x)$. A recurrence procedure for determining the successive approximations $\hat{E}^{(n)}(x)$ is developed in[5,6]. With the aim of practical construction of the wave field in a crystal with a dislocation, we henceforth confine ourselves in the expansion (2.5) to the first term $\hat{E}^{(n)}$ with $n = 0$. Then the fundamental equations of geometrical optics, namely the eikonal equation and the "transport" equation, take the following forms (see (2.2) and (2.5))

$$\left(\frac{\partial S}{\partial z} + \alpha(x)\right)^2 - \left(\frac{\partial S}{\partial x} - \alpha(x)\right)^2 = \tilde{\chi}^2, \tag{2.6}$$

$$\left(\frac{\partial}{\partial x} - \frac{\partial}{\partial z}\right)\hat{j} = 0, \quad \hat{j} = \sigma^2 \begin{pmatrix} \tilde{\chi}^2 - (\mathscr{D}_+ S)^2 \\ \tilde{\chi}^2 + (\mathscr{D}_+ S)^2 \end{pmatrix}, \tag{2.7}$$

$$\hat{E}^{(0)} = \sigma \begin{pmatrix} 0.5 C\chi_{-1} \\ \mathscr{D}_+ S \end{pmatrix},$$

where $\tilde{\chi} = 0.5\,|C|(\chi_{-1}\chi_1)^{1/2}$ (we shall henceforth omit the superscript 0 of $\hat{E}^{(0)}$ for the sake of simplicity).

The eikonal equation (2.6) is analogous to the one-dimensional relativistic Hamilton-Jacobi equation for particles with rest mass $\pm\tilde{\chi}$ in a certain variable external field. The only difference is that (2.6) and (2.7) contain the complex coefficient $\tilde{\chi} = \chi - i\gamma$, and consequently the trajectories and the eikonal are complex. Physically, this is connected with the damping of the x-ray wave field in the absorbing crystal. In the case of an arbitrary ratio of χ and γ, Eq. (2.6) is a system of two nonlinear equations with respect to the real and imaginary parts of the eikonal ($S = s + iq$). For x-rays we usually have $\gamma \ll \chi$. This enables us to regard the imaginary part of the eikonal as small in comparison with its real part. Putting $|q| \ll |s|$ and introducing the notation

$$-\frac{\partial}{\partial z}(s + iq) = H + i\Gamma, \quad \frac{\partial}{\partial x}(s + iq) = P + iQ, \tag{2.8}$$

we obtain from (2.6), accurate to terms of order $(q/s)^2 \sim (\gamma/\chi)^2 \ll 1$, the following equations for the determination of $s(x)$ and $q(x)$:

$$(H - \alpha)^2 - (P - \alpha)^2 = \chi^2, \tag{2.9}$$

$$(H - \alpha)\Gamma - (P - \alpha)Q = -\chi\gamma. \tag{2.10}$$

It is easily seen that the trajectory equations for the Hamilton-Jacobi equations (2.9) and (2.10) coincide and are given by

$$\frac{d}{dz}\left(\frac{\mp\chi\dot{x}}{\sqrt{1 - \dot{x}^2}}\right) = F(x), \tag{2.11}$$

where $\dot{x} = dx/dz$ and the "external force" $F(x)$ is determined by the derivative of the function $\alpha(x)$ in the propagation direction of the transmitted wave E_0:

$$F(x) = -\left(\frac{\partial}{\partial z} + \frac{\partial}{\partial x}\right)\alpha(x). \tag{2.12}$$

The minus and plus signs in (2.11) correspond respectively to x-rays that are weakly and strongly absorbed in the crystal. Equations equivalent to (2.11) and (2.12) were obtained in[9,10].

According to (2.8), the "transport" equation is also complex. In our case, when $\chi \gg \gamma$, the imaginary part of (2.7) can be neglected, since its inclusion introduces corrections of the order of γ/χ in the amplitudes E_0 and E_1. Thus, the "transport" equation takes the form

$$\frac{\partial}{\partial z}\{\sigma^2[\chi^2 + (P - H)^2]\} + \frac{\partial}{\partial x}\{\sigma^2[\chi^2 - (P - H)^2]\} = 0. \tag{2.13}$$

Formulas (2.8)–(2.13), and also (2.4), constitute the complete system of geometrical-optics equations describing the scattering of x-rays in distorted crystals in the general case of arbitrary smooth displacement fields $u(x)$. The partial differential equations (2.9) and (2.10) for the determination of the complex eikonal $S(x)$ can be expressed in the form of differential equations along the trajectories (2.11). Taking into account the connection between the usual momentum and the canonical momentum

$$p = P - \alpha(x), \quad p = \mp\chi\dot{x}/\sqrt{1 - \dot{x}^2}, \tag{2.14}$$

we obtain the sought equations for $s(x)$ and $q(x)$:

$$ds/dz = \pm\chi\sqrt{1 - \dot{x}^2} - \alpha(x)(1 - \dot{x}), \quad dq/dz = \mp\gamma\sqrt{1 - \dot{x}^2}. \tag{2.15}$$

The "transport" equation (2.13) admits, as usual, of formal integration along the ray trajectories

$$\sigma^2(x, z) = \sigma^2(x(z_1), z_1)\frac{1 + \dot{x}(z)}{1 + \dot{x}(z_1)}\left|\frac{\delta x(z_1)}{\delta x(z)}\right|. \tag{2.16}$$

Thus, the problem of the dynamic scattering of x-rays by static distortions of a crystal lattice reduces to the construction of the ray trajectories on which the wave field propagates in the crystal.

3. X-RAY SCATTERING BY THE ELASTIC FIELD OF A STRAIGHT-LINE DISLOCATION. GENERAL CASE

The elastic field $u_{i,j} = \partial u_i/\partial x_j$ of a straight-line dislocation in an infinite isotropic medium has the following invariant form[11,12]

$$u_{i,j} = -\frac{1}{4\pi\rho^2}\left\{2b_i n_j - 2m_i\rho_j + \frac{1}{1 - \nu}\left[m_i\rho_j + m_j\rho_i + D\left(\delta_{ij} - \tau_i\tau_j - \frac{2\rho_i\rho_j}{\rho^2}\right)\right]\right\}. \tag{3.1}$$

Here τ is a unit vector along the dislocation, $\rho = x - (x\tau)\tau$ is the distance from the point of observation in the crystal to the dislocation, $m = \tau \times b$, b is the Burgers vector, $n = \tau \times \rho$, $D = m \cdot \rho$, and ν is the Poisson coefficient.

Introducing the coefficient χ in the definition of the dimensionless coordinates x, z ($x = \kappa\chi X_1/\sin\theta$, $z = \kappa\chi X_3/\cos\theta$, where X_1 and X_3 are the absolute coordinates in the scattering plane (xOz), κ is the wave vector of the x-rays, and θ is the Bragg angle), and taking (2.3), (2.11), (2.12), and (3.1) into account, we obtain equations for the trajectories of the rays in a crystal with dislocation

$$\mp\ddot{x}/(1 - \dot{x}^2)^{3/2} = F(x, y, z), \tag{3.2}$$

$$F(x) = -\tfrac{1}{2}K_1\varkappa^{-2}(\cos^2\theta\, u_{1,33} - \sin^2\theta\, u_{1,11}). \tag{3.3}$$

The second-order differential equation (3.2) should be supplemented with two boundary conditions. We place the origin at the point of intersection of the dislocation with the x-ray scattering plane, which we take to be the plane $y = 0$. The customary boundary conditions for $x(z)$ are the values of the function and of its derivative at a point (x_1, z_1) on the upper surface of the crystal. In our case it is convenient to modify the boundary conditions, namely, we seek trajectories having a specified slope on the upper surface $z = z_1$ and passing through a given point $(x_0, 0)$ at the level $z = 0$:

$$x(0) = x_0, \quad \dot{x}(x_1, z_1) = \dot{x}_1 \quad (x_1 = x(z_1)). \tag{3.4}$$

The slope of the trajectories on the entrance surface is determined from the condition of continuity of the eikonal $S(x)$ at $z = z_1$. It follows from (2.4) that in the case of a plane wave incident on the crystal we have $S(x, z_1) = 0$. When (2.14) is taken into account, the initial slope of the trajectories is

$$\dot{x}(x_1, z_1) = \pm\alpha(x_1, z_1) / \sqrt{1+\alpha^2(x_1, z_1)}. \tag{3.5}$$

In the general case, the trajectories can be obtained by numerically integrating (3.2) subject to the boundary conditions (3.4) and (3.5). In the case of x-ray scattering by an elastic dislocation field (3.1), however, we can construct the trajectory field by successive approximations with respect to the parameter $\rho_0^{-1} \ll 1$, where $\rho_0 \approx x_0$ is the minimal distance of the trajectories from the core of the dislocation (in absolute units, $\rho_0 \gg \Lambda$). Indeed, it follows from (3.1) and (3.3) that the external force depends on the distance to the dislocation like

$$F(x, y, z) = h(x, y, z) / \rho^2, \tag{3.6}$$

where $h(x, y, z)$ is a function characterizing the angular dependence of the elastic field of the dislocation and is of the order of unity. At $\rho_0 \gg 1$ we have $|F_{max}| \sim \rho_0^{-2} \ll 1$, and a perturbation theory can be developed in terms of the parameter ρ_0^{-1}. The iteration procedure of constructing the solution of the boundary-value problem (3.2)–(3.5) with allowance for (3.6) reduces to the following: In first-order approximation

$$\mp \ddot{x}^{(1)}(z) = 0, \quad \dot{x}^{(1)}(z_1) = 0, \quad x^{(1)}(0) = x_0; \tag{3.7}$$

In second-order approximation

$$\mp\ddot{x}^{(2)}(z) = F(x^{(1)}(z), z), \quad \dot{x}^{(2)}(z_1) = \pm\alpha(x^{(1)}, z_1), \quad x^{(2)}(0) = 0 \tag{3.8}$$

etc. It is easy to see that the higher approximations introduce corrections on the order of ρ_0^{-1} and higher in the trajectories.

The successive-approximation equations determine the trajectory field in the x-ray scattering plane at $\rho_0 > 1$. We note that the equations of the first two approximations correspond to nonrelativistic particle motion. Allowance for relativistic corrections (the term $\ddot{x}\dot{x}^2$ in (3.2)) is essential starting with the fourth-order approximation.

Integrating (3.7) and (3.8) in succession, we obtain the ray trajectories accurate to terms of order ρ_0^{-1}:

$$x(z) \approx x_0 + x^{(2)}(z) \equiv x_0 \mp x_d(z) = x_0 \mp \int_{z_0}^{z} dz' \int_{z_1}^{z'} dz'' F(x_0, z'') \pm (z-z_0)\,\alpha(x_0, z_1). \tag{3.9}$$

Formal substitution of (3.9) in (2.15) and (2.16) leads to the following expressions for the x-ray field in a crystal with a dislocation:

$$\hat{E}(x(z_2), z_2) = \exp\{i\chi_0(z_2 - z_1)/2\chi\}$$
$$\times \Big[\mathcal{R}_-(z_1, z_2)\left(1 - \frac{\dot{x}_d(z_2) - \dot{x}_d(z_1)}{2}\right)\sigma_0^- \begin{pmatrix} 0{,}5C\chi_{-1}/\chi \\ 1 + \dot{x}_d(z_2) \end{pmatrix} e^{iS(x_2, z_2, z_1)}$$
$$+ \mathcal{R}_+(z_1, z_2)\left(1 + \frac{\dot{x}_d(z_2) - \dot{x}_d(z_1)}{2}\right)\sigma_0^+ \begin{pmatrix} 0.5C\chi_{-1}/\chi \\ -1 + \dot{x}_d(z_2) \end{pmatrix} e^{-iS(x_2, z_2, z_1)}\Big],$$

$$\mathcal{R}_\pm(z_1, z_2) = \left|\frac{1 \pm J(z_1)}{1 \pm J(z_2)}\right|^{1/2}, \quad J(z) = \frac{\delta x_d(z)}{\delta x_0}, \tag{3.10}$$

$$S(x_2, z_2, z_1) = \left(1 - \frac{i\gamma}{\chi}\right)\left(z_2 - z_1 - \frac{1}{2}\int_{z_1}^{z_2} dz\, \chi_d^2(z)\right)$$
$$+ \int_{z_1}^{z_2} dz\left[x_d(z)\frac{\partial\alpha(x_0, z)}{\partial x_0} - \dot{x}_d(z)\,\alpha(x_0, z)\right]. \tag{3.11}$$

In (3.10) and (3.11), the x-ray field is determined accurate to a phase factor. We note that the next higher terms in the expansion

$$x(z) = \sum_{n=1}^{\infty} x^{(n)}(z)$$

would lead to the appearance of terms with ρ_0^{-1} raised to the third and higher powers in the eikonal and in the amplitudes.

Thus, formulas (3.9)–(3.11), and also (3.1) and (3.3), solve the problem of the scattering of x-rays by a dislocation within the framework of geometrical optics, and make it possible to construct the wave field along trajectories whose minimum distance from the core of the dislocation is $\rho_0 \approx |x_0| > 1$.

By way of example, we shall consider below the scattering of x-rays by a dislocation under anomalous transmission conditions, when $\min(|z_1|, z_2) > \mu_0^{-1}$.

4. EDGE DISLOCATION PERPENDICULAR TO THE X-RAY SCATTERING PLANES. THE BORRMANN CASE

Under dynamic scattering conditions, when the sample thickness $t \gg \mu_0^{-1}$, a Borrmann x-ray wave field propagates in the crystal. The contribution of the strongly absorbed x-rays (the plus sign in (3.2)) can then be disregarded in the scattering picture.

Assume that the crystal contains an edge dislocation perpendicular to the scattering plane, with a Burgers vector $\mathbf{b} \parallel \mathbf{K}_1$. In accordance with (3.1), the distortion components $u_{1,1}$ and $u_{1,3}$, which determine the local deviation $\alpha(\mathbf{x})$ from the Bragg condition, are equal to

$$u_{1,1} = \frac{bX_3}{4\pi(1-\nu)(X_1^2+X_3^2)}\left(2\nu - 1 - \frac{2X_1^2}{X_1^2+X_3^2}\right),$$
$$u_{1,3} = \frac{bX_1}{4\pi(1-\nu)(X_1^2+X_3^2)}\left(3 - 2\nu - \frac{2X_3^2}{X_1^2+X_3^2}\right). \tag{4.1}$$

Substituting (4.1) in (3.3) and taking (3.9) into account, we obtain the trajectories of the weakly absorbed x-rays:

$$x(z) - x_0 = \frac{G}{2(1-\nu)}\left[C_1\xi + \left(A + \frac{B}{2}\right)\operatorname{arctg}\xi + \frac{B\xi}{2(1+\xi^2)}\right], \tag{4.2}$$

where

$$G = \frac{K_1 b}{2\pi}, \quad A = 2\nu - 1 + \frac{1+2\nu}{k^2} \quad B = -2\left(1 + \frac{1}{k^2}\right),$$
$$k = \operatorname{ctg}\theta, \quad \xi = \frac{kz}{x_0}, \tag{4.3}$$
$$C_1 = \frac{k^{-1} - \xi_1}{k(1+\xi_1^2)}\left(1 - 2\nu + \frac{2}{1+\xi_1^2}\right) - \frac{2}{k^2(1+\xi_1^2)}.$$

The shapes of the trajectories become much simpler in those regions of variation of the argument ξ where $|\xi_2|, |\xi_1| \gg 1$ and $|\xi_2|, |\xi_1| \ll 1$ (nearby and remote trajectories, respectively). Thus, at $|\xi_2|, |\xi_1| \ll 1$, corresponding to longitudinal distances from the dislocation axis that are much larger than the crystal thickness, we have

$$x - x_0 \approx \frac{G\xi}{2(1-\nu)}\left(A + B + \frac{1-2\nu}{k^2}\right) \tag{4.4}$$

and the ray trajectories are straight lines, $x = x_0$, accurate to $|\xi| \ll 1$. In the opposite limiting case, when $|\xi_2|, |\xi_1| \gg 1$, the trajectories flow around the core of the dislocation and then rapidly straighten out, thereby experiencing a finite longitudinal displacement

$$\Delta x = x_2 - x_0 \approx \frac{G}{2(1-\nu)}\left[\frac{2\nu - 1}{k}\frac{z_2}{z_1} + \frac{\pi}{2}\left(A + \frac{B}{2}\right)\right]. \tag{4.5}$$

The trajectories of weakly absorbed x-rays in a crystal with a dislocation, constructed in accordance with the general formulas (4.2) and (4.3), are shown in Fig. 1.

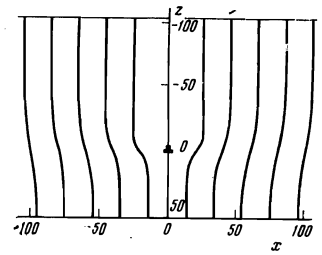

FIG. 1. Trajectories of weakly absorbed x-rays scattered by an edge dislocation perpendicular to the scattering plane.

Expressions (4.1)–(4.3) permit a direct integration of the equations along the trajectories (2.15) and (2.16) for the eikonal $S(x)$ and the amplitude $\hat{E}(x)$ of a Borrmann wave field. It is easily seen that the explicit form of the real part of the eikonal is immaterial for determination of the intensity of the scattered radiation (see (3.10) and (3.11), where the wave field of the strongly absorbed x-rays can be neglected).

Substituting (4.1)–(4.3) in (2.15), (2.16), (3.10), and (3.11), we obtain expressions for the imaginary part of the eikonal $q(x)$ and for the amplitude $\hat{E}(x)$:

$$q(x, z) = w(x, z) - w(x_1, z_1),$$

$$w(x,z) = -\frac{1}{2\chi}\gamma z + \frac{k\gamma G^2}{4\pi\chi(1-\nu)^2 x_0}\left\{C_1{}^2\xi + \left(\frac{1}{2}A^2 + \frac{5}{16}B^2 + \frac{3}{4}AB + 2AC_1 + BC_1\right)\operatorname{arctg}\xi + \frac{\xi}{2(1+\xi^2)}\left[A^2 + \frac{5}{8}B^2 + \frac{3}{2}AB + 2BC_1 + \left(AB + \frac{5}{12}B^2\right)\frac{1}{1+\xi^2} + \frac{B^2}{3(1+\xi^2)^2}\right]\right\}, \tag{4.6}$$

$$\hat{E}(x, z) = \sigma_0^-\begin{pmatrix} 0{,}5C\chi_{-1}/\chi \\ 1 + \dot{x}_d(z)\end{pmatrix}\left(1 - \frac{\dot{x}_d(z) - \dot{x}_d(z_1)}{2}\right)\mathcal{R}_-(z_1, z) \times \exp\left\{-\frac{\chi_0''}{2\chi}(z - z_1) - q(x, z)\right\}. \tag{4.7}$$

If $|\xi_1|, |\xi| \gg 1$ (nearby trajectories), we obtain

$$q(x, z) = -\frac{\gamma}{2\chi}(z - z_1) + \frac{g\gamma}{2|x_0|\chi}, \tag{4.8}$$

$$g = \frac{\pi k G^2}{4(1-\nu)^2}\left(\frac{1}{2}A^2 + \frac{5}{16}B^2 + \frac{3}{4}AB + 2AC_1 + BC_1\right),$$

$$\hat{E}(x, z) = \sigma_0^-\begin{pmatrix} 0.5C\chi_{-1}/\chi \\ 1\end{pmatrix}\exp\left\{-\frac{\chi_0''(z - z_1)}{2\chi} - q(x, z)\right\}. \tag{4.9}$$

It follows from (4.6)–(4.9) that the intensity of the x-rays scattered by the dislocation under conditions of normal transmission behave in the following manner. Behind the dislocation, in the region $|x_2| < \gamma_g\chi^{-1}$, there is produced a shadow whose width does not depend on the crystal thickness. The intensity of the transmitted and diffracted waves varies exponentially:

$$I_{0,1}(x_2) \sim \exp(-\gamma g|x_2 - \Delta x|^{-1}). \tag{4.10}$$

The change in the local density of the trajectories $|\delta x_1/\delta x_2|$ is negligibly small (a nearly uniform trajectory distribution is established at large distances from the dislocation core) and does not influence the contrast of the dislocation.

Figure 2 shows the intensity distributions $I_{0,1}(x_2)$ plotted in accord with the obtained formulas for anomalous-transmission conditions. We assumed in the calculations $\theta = 22°30'$, $\gamma = +0.04\chi$, $z_1 = -100$, $z_2 = 50$ (Ge single crystal, $\mu_0 t = 6$, reflection (220), MoK_α radiation). We see that the character and dimension of the shadow are determined completely by the exponential factor $\exp(-q(x_2))$. A similar structure of the Borrmann image was observed experimentally[13]. The general form of the $I_{0,1}(x_2)$ curve is adequately described qualitatively by the asymptotic expressions (4.8)–(4.10).

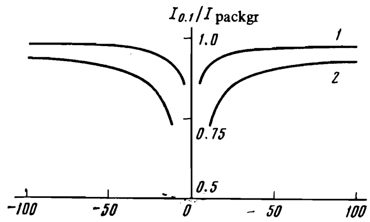

FIG. 2. Intensities $I_0(x_2)$ and $I_1(x_2)$ of the transmitted and diffracted waves, respectively, scattered by an edge dislocation perpendicular to the scattering plane under anomalous-transmission conditions: 1—Burgers vector **b** = (1/2)[110], G = 2; 2—**b** = [110], G = 4.

Thus, within the framework of geometric optics we can construct the wave field of x-rays scattered by a dislocation. The limits of applicability of the considered geometrical-optics approximation coincide with the conditions for the smallness of the "relativism" parameter for a particle moving along a trajectory, namely $\dot{x}^2 \ll 1$. Violation of this condition occurs in a narrow region of impact parameters $|x_0| \lesssim 1$. To estimate the intensity of the scattered x-rays which do not satisfy the criterion for the applicability of geometrical optics, one can use the influence-function method[6].

It turns out[6] that the scattering of the Borrmann wave field propagating in a narrow region $|x_0| \lesssim 1$ must be taken into account when the distance from the dislocation to the lower surface of the crystal is smaller than the photoelectric-absorption length, i.e., $\mu_0 z_2 < 1$. This gives rise to interference bands (the so-called Pendellosung), the form of which is determined by the influence functions. If $\mu_0 z_2 > 1$, as in our problem, the interference bands vanish and the picture of the dynamic scattering of x-rays by a dislocation can be adequately described in the geometrical-optics approximation.

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