Dynamic scattering of x rays in a crystal with a constant deformation gradient

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Using the exact solution of the problem of dynamic scattering of x rays in a crystal with a constant strain gradient, we construct the quasiclassical asymptotic form of the wave field for a wide range of scattering parameters and calculate the pre-exponential factor as a function of the crystal deformation B. The divergence of the integral intensity of the scattered wave for a nonabsorbing crystal, which is known from the theory of geometric optics in the limiting case $|B|\gg 1$, is lifted in this case because of the static scattering factor (pre-exponential factor) of the form $1-\exp(-\pi/2|B|)$. The limits of applicability of geometrical optics are determined on the basis of the trajectory approach. The qualitative features of dynamic scattering of x rays by an elastically bent crystal, particularly the formation of the caustic and the focusing of the x rays are determined.

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1. INTRODUCTION

Until recently, it was customary to use the theory of geometric optics to analyze the dynamic scattering of x rays in an inhomogeneous crystal.[1-6] In the case $l_{\rm eff} \gg \Lambda$, where $l_{\rm eff}$ is the characteristic inhomogeneity length of the crystal and Λ is the scattering length (the extinction length) for radiation in a perfect crystal, the first term of the asymptotic series of the expansion obtained within the framework of this theory in powers of $\Lambda l_{\rm eff}^{-1} \ll 1$ gives the correct result. If, however, $l_{\rm eff} \lesssim \Lambda$, then all the terms of the series become of the same order, and the geometric-optics theory leads to qualitatively incorrect conclusions.

It is known (see, e.g.,[7]) that a general method of solving scattering problem is to construct the quasiclassical asymptotic wave function on the basis of trajectories corresponding to the classical equations of motion. The effectiveness of this approach, if it can be used consistently, is obvious, for in the general case the multidimensional scattering problem reduces to one-dimensional, and the essential singularities of the scattering, where the quasiclassical approximations are violated, have the clear-cut physical meaning of formation of caustics.

The principal role is assumed in this connection by the class of problems of dynamic scattering of x rays (DXRS) in an inhomogeneous crystal with a constant strain gradient. It turns out that in this case the boundary-value scattering problem can be solved exactly[8-11] (see also[12, 13]). In[9, 11] there was constructed a retarded Green-Riemann function for x-ray quanta in a crystal with an elastic-displacement field that is an arbitrary quadratic function of the coordinates in the scattering plane. An investigation of the solution obtained there is of interest in itself, since it permits a complete analysis of the problem of quasiclassical scattering of particles (x-ray quanta) in the case of a "potential" that is a linear function of the coordinates.

The present paper is devoted to an investigation of the quasiclassical approximation in the two-dimensional DXRS problem in the case of a homogeneous strain gradient. Special attention is paid to the calculation of the pre-exponential factor of the quasiclassic asymptotic wave field as a function of the crystal deformation. In Sec. 2, to solve the boundary-value problem, an oblique dimensionless coordinate system is introduced, in which the mathematical formulation of the problem and the analysis of the result become much simpler. A complete system of influence functions of a point source (Green's functions) is obtained, and an integral formulation is presented of the Huyghens-Fresnel principle for a wave field in a crystal. In Sec. 3 we present a detailed analysis and construct the asymptotic Green's function in a wide range of the parameters of the scattering problem close to (the wave region) and far from (the quasiclassical region) the characteristics of the influence region of a pointlike source. In the region where the quasiclassical approximation is valid, we obtain the static scattering factor and the scattering phase shift (the two together constitute the pre-exponental factor) as functions of the effective deformation of the crystal B. This procedure eliminates automatically the divergence, known from the theory of geometric optics and linear in $|B| \gg 1$, of the integrated (over the angles) intensity of the scattered wave for a non-absorbing crystal. At low effective deformations $|B| \ll 1$, the regions of applicability of the wave and of the quasiclassical approximations overlap and it becomes possible to obtain a simple interpolation formula for the Green's function in the entire influence region. The quasiclassical approximation is used (Sec. 4) to reveal the qualitative features of the propagation of x rays in an elastically bent crystal. It is interesting that the spatial distribution of the wave field of an incident plane wave passing through such a crystal exhibits a number of characteristic features of energy focusing of x rays with formation of caustics. Using symmetrical DXRS as an example, we demonstrate the feasibility, in principle, of using a bent crystal as a lens for x rays, starting with a certain crystal thickness. The focal length is determined and an equation is obtained for the caustics.

2. FORMULATION OF PROBLEM

When an x-ray beam is incident on a crystal oriented near the regular Bragg reflection, the wave field inside the crystal is a coherent superposition of a transmitted wave and a scattered wave' this superposition is described by the Takagi system of dynamic equations.[14-16, 3, 5, 9] In a form symmetric with respect to the amplitudes

$$\mathscr{E}_{0,1}=\exp\left\{iK\left(\frac{\chi_0}{2\gamma_0}s_0+\frac{\chi_0-\alpha}{2\gamma_1}s_1\right)\right\}E_{0,1}, \tag{2.1a}$$

these equations become

$$i\frac{\partial E_0}{\partial s_0}+\frac{\pi}{\Lambda}\sigma_{-1}\exp(i\mathbf{hu}(\mathbf{R}))E_1=0,$$
$$i\frac{\partial E_1}{\partial s_1}+\frac{\pi}{\Lambda}\sigma_1\exp(-i\mathbf{hu}(\mathbf{R}))E_0=0. \tag{2.1b}$$

Here $\mathbf{h}$ is the reciprocal-lattice vector multiplied by 2π, $\mathbf{u}(\mathbf{R})$ is the vector of elastic displacement at the point $\mathbf{R}$, the oblique coordinate system with axes along the directions $\mathbf{K}_0$ of the incident beam and $\mathbf{K}_1$ of the scattered beam is defined by the relation

$$\mathbf{R}=\frac{\mathbf{K}_0}{K\gamma_0}s_0+\frac{\mathbf{K}_1}{K\gamma_1}s_1, \tag{2.2}$$

where γ_0 and γ_1 are the direction cosines, $\gamma_{0,1} = \cos(\widehat{\mathbf{K}_{0,1}\mathbf{n}})$, $\mathbf{n}$ is the inward normal to the entrance surface of the crystal, $K = \omega/c$, ω is the frequency of the x-ray wave, and c is the speed of light. The dynamic coefficients $\sigma_{\pm1}$ are accordingly defined by the formulas

$$\sigma_{-1}=\frac{\Lambda}{\pi}\frac{\mathscr{C}K\chi_{-1}}{2\gamma_0}=\frac{1}{\sqrt{|\beta|}}\left(\frac{\chi_{-1}}{\chi_1}\right)^{1/2}(1+ik),$$
$$\sigma_1=\frac{\Lambda}{\pi}\frac{\mathscr{C}K\chi_1}{2\gamma_1}=\frac{\beta}{\sqrt{|\beta|}}\left(\frac{\chi_1}{\chi_{-1}}\right)^{1/2}(1+ik), \tag{2.3}$$

where χ_0 and $\chi_{\pm1}$ are the Fourier components of the polarizability of the crystal, Λ is the extinction length, $\mathscr{C}$ is a polarization factor equal to unity or to $\cos 2\theta$, $k = (\chi_1'\chi_{-1}'' + \chi_{-1}'\chi_1'')/2\Psi$ is the normalized dynamic absorption coefficient, $\Psi = \chi_1'\chi_{-1}' - \chi_1''\chi_{-1}''$, a single prime denotes the real part and a double prime the imaginary part of the corresponding quantity, and $\beta = \gamma_0/\gamma_1$. We note that by definition $k < 0$ and usually $|k| \ll 1$.

The system (2.1b) has been written out in the oblique system (s_0, s_1), but the boundary conditions are formulated on the entrance surface of the crystal. It is therefore expedient to introduce a dimensionless "special" system of coordinates (see Fig. 1) with the aid of the relations

$$z=\frac{\pi}{\Lambda}Z=\frac{\pi}{\Lambda}(s_0+s_1),\quad x=\frac{\pi}{\Lambda}(s_0-s_1). \tag{2.4}$$

It is easily seen that the x axis coincides in direction with the Cartesian axis X, and the z axis is the median of the triangle made up by the axes s_0, s_1, and d (Fig. 1), since

$$Z=\frac{2\gamma_0\gamma_1}{\sin(2\psi)}X$$

at $x = 0$. Here $\psi = (\varphi_0 + \varphi_1)/2$ is the angle between the bisector of the angle s_1Os_0 and the Z axis.

We note that in the chosen coordinate system (x, z) the mathematical formulation of the problem, in the general case of asymmetric scattering, is of the same form as the formulation in the symmetric case (see, e.g.,[5]). This circumstance greatly simplifies the analysis.

In the DXRS case in a crystal with a constant strain gradient, the function $\mathbf{h}\cdot\mathbf{u}(\mathbf{R})$ is quadratic in the coordinates

$$\mathbf{hu}(\mathbf{R})=2\frac{\pi^2}{\Lambda^2}(As_0^2+2Bs_0s_1+Cs_1^2). \tag{2.5}$$

For the same of simplicity, we have left out from the expression for the displacement field $\mathbf{u}(\mathbf{R})$ in (2.5) the terms that are linear in the coordinates, since allowance for them leads only to a renormalization of the value of the Bragg scattering angle θ. Expressions for the displacement-field components in the case of mechanical and temperature flexures are given in[17,1].

In the (x, z) system, the boundary-value problem is formulated as follows (see (2.1) and (2.4)):

$$\mathscr{E}_{0,1}(\mathbf{r})=\exp(i\eta\mathbf{r})E_{0,1}(\mathbf{r});\quad \eta_{x,z}=\frac{\chi_0(1\mp\beta)\pm\alpha\beta}{2\mathscr{C}\sqrt{|\beta|\Psi}}, \tag{2.6a}$$

$$\begin{pmatrix} i\left(\frac{\partial}{\partial z}+\frac{\partial}{\partial x}\right) & \sigma_{-1}\exp(i\mathbf{hu}) \\ \sigma_1\exp(-i\mathbf{hu}) & i\left(\frac{\partial}{\partial z}-\frac{\partial}{\partial x}\right)\end{pmatrix}\begin{pmatrix}E_0\\E_1\end{pmatrix}=0, \tag{2.6b}$$

$$\mathscr{E}_0(x,0)=\mathscr{E}(x),\quad \mathscr{E}_1(x,0)=0, \tag{2.7}$$

where the displacement-field function $\mathbf{h}\cdot\mathbf{u}$ in (2.6b) is of the form (2.5).

We note that η_X' is the normalized angular deviation from the exact Bragg condition. The imaginary part, η_X'', describes in the general case ($\beta \neq 1$) the asymmetry of the absorption of the x-ray beam in the crystal.

The solution of the problems (2.5) and (2.6) can be obtained with the aid of the Riemann method or with the retarded Green's function $\mathfrak{G}(x_P, x, z_P, z)$[10,11]. Using the influence functions of a pointlike source obtained in there under the DXRS conditions, for any point (x_P, z_P) of the triangular region bounded by the contour L and by the characteristics drawn from its ends to the point (x_P, z_P) (Fig. 2), we define the amplitudes of the transmitted and scattered waves by the expressions

$$\mathscr{E}_0(P)=\int_{RQ}\mathfrak{G}_{00}(x_P,x,z_P,z)\mathscr{E}_0(x,z)\,(dx-dz)+\int_{RQ}\mathfrak{G}_{01}(x_P,x,z_P,z)\mathscr{E}_1(x,z)\,(dx+dz), \tag{2.8a}$$

$$\mathscr{E}_1(P)=\int_{RQ}\mathfrak{G}_{10}(x_P,x,z_P,z)\mathscr{E}_0(x,z)\,(dx-dz)+\int_{RQ}\mathfrak{G}_{11}(x_P,x,z_P,z)\mathscr{E}_1(x,z)\,(dx+dz). \tag{2.8b}$$

The influence functions take here the form

$$\begin{aligned}
\mathfrak{G}_{00}(\mathbf{r}_P,\mathbf{r})&=\exp\{i\eta(\mathbf{r}_P-\mathbf{r})+iS_0\}\Big\{\delta(x-x_P+z_P-z-0)\\
&\quad-\frac{\sigma^2}{4}(z_P-z+x_P-x)\,{}_1F_1\left(1+i\frac{\sigma^2}{4B},2;\ iB\rho^2\right)\Big\},\\
\mathfrak{G}_{10}(\mathbf{r}_P,\mathbf{r})&=\frac{i\sigma_1}{2}\exp\{i\eta(\mathbf{r}_P-\mathbf{r})+iS_0-i(\mathbf{hu})_P\}\,{}_1F_1\left(1+i\frac{\sigma^2}{4B}\ 1;\ iB\rho^2\right),\\
\mathfrak{G}_{11}(\mathbf{r}_P,\mathbf{r})&=\exp\{i\eta(\mathbf{r}_P-\mathbf{r})-iS_1\}\Big\{\delta(x-x_P+z-z_P+0)\\
&\quad-\frac{\sigma^2}{4}(z_P-z-x_P+x)\,{}_1F_1\left(1-i\frac{\sigma^2}{4B},\ 2;\ -iB\rho^2\right)\Big\}\\
\mathfrak{G}_{01}(\mathbf{r}_P,\mathbf{r})&=\frac{i\sigma_{-1}}{2}\exp\{i\eta(\mathbf{r}_P-\mathbf{r})-iS_1+i(\mathbf{hu})_P\}\,{}_1F_1\left(1-i\frac{\sigma^2}{4B}\ 1;\ -iB\rho^2\right)
\end{aligned} \tag{2.9}$$

where ${}_1F_1(a, b; x)$ is a confluent hypergeometric function,

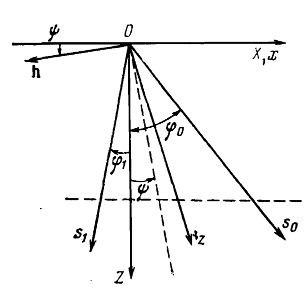

FIG. 1

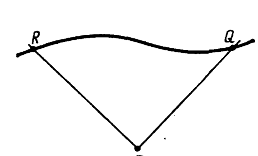

FIG. 2

FIG. 1. Scattering geometry. The positive direction of the angles is counterclockwise.
FIG. 2. Influence region for the observation.

$\rho^2 = (z_P - z)^2 - (x_P - x)^2$, $\sigma^2 = 1 + 2ik$, $S_{0,1}$ are quadratic functions of the coordinates, equal to

$$S_0(\mathbf{r}_P, \mathbf{r}) = {}^1/_2 C[(z_P - x_P)^2 - (z - x)^2] + {}^1/_2 B[(z_P + x)^2 - (x_P + z)^2 - \rho^2],$$
$$S_1(\mathbf{r}_P, \mathbf{r}) = {}^1/_2 A[(z_P + x_P)^2 - (z + x)^2] + {}^1/_2 B[(z_P - x)^2 - (z - x_P)^2 - \rho^2]. \tag{2.10}$$

In (2.9) the symbols ± 0 ensure that the singular point of the δ-function will fall in the integration region.

The general relations (2.8) together with formulas (2.9) constitute the Huyghens-Fresnel principle in the Kirchhoff form under the DXRS conditions in a crystal with a constant strain gradient. On going to a perfect crystal, when the coefficients A, B, and C tend to zero, the influence functions can be readily shown to go over into the corresponding expressions for a perfect crystal.[5] We note that, as seen from (2.9), the influence functions are, apart from a phase factor, invariant to translations. Physically this is connected with the invariance of the distribution of the intensity of a pointlike source placed in a homogeneously bent crystal, with respect to translations that constitute a superposition of two pairs of successive rotations through equal and opposite angles relative to the center of curvature of the reflecting planes (center of curvature of the neutral plane) and the point at which the source is located. In each of these rotations, the intensity of the diffraction image of the source, which is equal to the square of the modulus of the influence function, depends only on the difference of the coordinates of the source and of the observation point.

In an x-ray experiment the source is usually placed on the z = 0 surface of the crystal. Then, taking into account the boundary conditions (2.7), we obtain for the amplitudes of the transmitted and scattered waves (cf. (2.8))

$$\mathscr{E}_0(P) = \int_{RQ} dx\, \mathfrak{G}_{00}(x_P, x, z_P, 0)\mathscr{E}(x),$$
$$\mathscr{E}_1(P) = \int_{RQ} dx\, \mathfrak{G}_{10}(x_P, x, z_P, 0)\mathscr{E}(x). \tag{2.11}$$

Expressions (2.8), (2.11), and also (2.9), (2.10), in accord with the Huyghens-Fresnel principle, solve completely the problem of x-ray optics of a crystal with a constant strain gradient.

It is interesting that if the axis of the homogeneous bending of the crystal lies in a reflecting plane, then $B = 0$, $A \neq 0$, $C \neq 0$, and the influence functions coincide, accurate to within a phase factor, with the corresponding expressions for a perfect crystal. In this case the integrated (over the angles) intensity of the scattered wave R_i, which can be easily shown to equal

$$R_i = \int_{-z_P}^{z_P} dx |\mathfrak{G}_{10}|^2,$$

does not depend on the magnitude of the strain.

Further investigations of the solutions (2.8) and (2.11) call for the use of nonstandard asymptotic expansions of the confluent hypergeometric function ${}_1F_1$ as a function of the effective deformation parameter B. This question will be discussed in detail below.

3. THE ASYMPTOTIC GREEN'S FUNCTIONS

The spatial distribution of the wave field in the crystal is determined, in accord with the Huyghens-Fresnel principle (28), by the influence functions of the pointlike source (2.9) (the Green's functions). It is obvious that in physical applications the effective expansions of the Green's functions are those in powers of the deformation of the crystal. To obtain Green's-function representations of interest to us for a wide range of parameters of the problem and of the argument, we use Olver's method.[18]

The gist of the method is to construct an asymptotic form of the Whittaker function

$$F(t) = \exp(-2i\varepsilon\varkappa t)(4i\varepsilon\varkappa t)^{b/2}{}_1F_1(b/2 + i\varepsilon\varkappa,\, b;\, 4i\varepsilon\varkappa t), \tag{3.1}$$

where

$$t = \frac{B^2\rho^2}{\sigma^2}, \quad \varkappa = \frac{\sigma^2}{4|B|} = \frac{1+2i\bar{k}}{4|B|}, \quad \bar{k} = k + B(b-2), \quad \varepsilon = \operatorname{sign} B.$$

We introduce a function W(v) defined by

$$W(v) = (dt/dv)^{-1/2}F(t),$$

where the new variable v is defined by the relation

$$v(t) = i\frac{\varkappa}{|\varkappa|}\{\sqrt{t(1+t)} - \ln(\sqrt{1+t} - \sqrt{t})\}. \tag{3.2}$$

The function W(v) satisfies the equation

$$d^2W/dv^2 = \{4|\varkappa|^2 + f(v)\}W, \tag{3.3}$$

whose two linearly-independent solutions have, in accordance with Olver's theorem, the asymptotic expansions

$$W_1 = \exp(2|\varkappa|v)\left[\sum_{s=0}^{M-1}\frac{A_s(v)}{(2|\varkappa|)^s} + 0((2|\varkappa|)^{-M})\right],$$
$$W_2 = \exp(-2|\varkappa|v)\left[\sum_{s=0}^{M-1}\frac{(-1)^s A_s(v)}{(2|\varkappa|)^s} + 0((2|\varkappa|)^{-M})\right]. \tag{3.4}$$

Here the functions $A_s(v)$ are determined by the recurrence relations

$$A_{s+1}(v) = -\frac{1}{2}\frac{dA_s(v)}{dv} + \frac{1}{2}\int f(v)A_s(v)dv + K_s, \quad A_0 = 1, \tag{3.5}$$

K_s is an arbitrary constant, which is conveniently chosen such that $A_s(v) \to 0$ as $v \to \infty$. The function f(v) is in our case equal to

$$f(v) = \left(\frac{dt}{dv}\right)^2\frac{b(b-2)}{4t^2} - \left[3\left(\frac{d^2t}{dv^2}\right)^2 - 2\frac{dt}{dv}\frac{d^3t}{dv^3}\right] \Big/ 4\left(\frac{dt}{dv}\right)^2. \tag{3.6}$$

We note that the function v(t) has the meaning of a complex eikonal, as follows from (3.4), and in principle can be obtained by the method of complex trajectories. On the other hand it is clear that it is possible to construct a quasiclassical asymptotic form of the wave field by going over directly in the initial system of equation (2.1b) to one action variable along the classical trajectory.

Using the linear connection between the functions W, W_1, and W_2 and also the asymptotics of these functions at large values of the argument, we obtain for ${}_1F_1$ the following representation:

$${}_1F_1 = \Gamma(b)\exp(2i\varepsilon\varkappa t)(4\varkappa t)^{-b/2}[t/(1+t)]^{1/4}$$
$$\times\left\{\frac{(-i\varkappa)^{-i\varkappa}\exp(i\varkappa + i\pi b/4)}{\Gamma(b/2 - i\varkappa)}W_2 + \frac{(i\varkappa)^{i\varkappa}\exp(-i\varkappa - i\pi b/4)}{\Gamma(b/2 + i\varkappa)}W_1\right\}, \tag{3.7}$$

where $\Gamma(z)$ is the Gamma function. Physically, the representation of the Green's function of an x-ray point source in the form of a sum of two terms corresponds to the propagation in the crystal of two wave fields (in accord with the two branches of the dispersion surface

$\omega_{1,2}(\mathbf{K}) = \omega$),[10] with W_1 and W_2 corresponding to weakly and strongly absorbed waves, respectively.

A direct analysis of expressions (3.2) and (3.4)–(3.6) shows that the region of applicability of the quasiclassical expansions (3.4) has a limit not stronger than

$$\rho \gg 1, \tag{3.8}$$

independently of the degree of deformation of the crystal. This means that when the condition (3.7) is satisfied we can confine ourselves in (3.7) in practice to the first nonvanishing terms of the series (3.4). In the opposite limiting case, namely near the characteristic rays $z = \pm x$ (the wave region), the function ${}_1F_1$ can be represented in the form of Olver's third asymptotic expansion[18]:

$$\begin{gathered}{}_1F_1(b/2+i\varepsilon\varkappa, b; 4i\varepsilon\varkappa t) \sim \Gamma(b)\exp(2i\varepsilon\varkappa t)\\ \times(2|\varkappa|\sqrt{t})^{1-b}\left\{J_{b-1}(4|\varkappa|\sqrt{t})\left[\sum_{s=0}^{N-1}\frac{A_s(2\sqrt{i\varepsilon\varkappa t})}{(4i\varepsilon\varkappa)^s}+0((4i\varepsilon\varkappa)^{-N})\right]\right.\\ \left.+\frac{1}{2\sqrt{-i\varepsilon\varkappa}}J_b(4|\varkappa|\sqrt{t})\left[\sum_{s=0}^{N-1}\frac{B_s(2\sqrt{i\varepsilon\varkappa t})}{(4i\varepsilon\varkappa)^s}+0((4i\varepsilon\varkappa)^{-N})\right]\right\}.\end{gathered}\tag{3.9}$$

The functions A_s and B_s are connected and defined in analogy with (3.5) (for more details see[18]). The region of applicability of the representation (3.9) depends on the degree of deformation of the crystal' at large (small) $|\kappa|$, i.e., small (large) values of the deformation parameter B, the expansion is respectively in powers of $4|\kappa|t^{3/2}$ and $t^{1/2}$.

We note that formulas (3.7) and (3.9) are valid in the general case of an arbitrary deformation gradient B, the value of which determines in turn the region of applicability of the expansions obtained for the Green's functions.

Formula (3.7) can be greatly simplified if it is recognized that for x rays the dynamic absorption coefficient is usually $|\mathbf{k}| \ll 1$. The expression for the function $v(\rho)$ in the region of applicability of (3.8) then takes the form

$$\begin{gathered}v(\rho)=iS(\rho)-\frac{2\tilde{k}}{4|B|}-i\frac{1+2i\tilde{k}}{4|B|}\ln(1+2i\tilde{k}),\\ S(\rho)=\frac{\rho}{2}\sqrt{1+B^2\rho^2}-\frac{1+2i\tilde{k}}{2|B|}\ln(\sqrt{1+B^2\rho^2}-|B|\rho).\end{gathered}\tag{3.10}$$

As a result we obtain after direct simplifications

$$\begin{gathered}{}_1F_1\sim\Gamma(b)\exp(iB\rho^2/2)(|B|\rho^2)^{(1-b)/2}\{C_+(\varepsilon, b, |B|)\\ \times\exp(iS(\rho))+C_-(\varepsilon, b, |B|)\exp(-iS(\rho))\},\end{gathered}\tag{3.11a}$$

$$C_+(\varepsilon)=C_-^*(-\varepsilon)=\frac{(i/4|B|)^{i/4|B|-\varepsilon(b-2)/2}\exp(-i/4|B|-i\pi b/4)}{\Gamma(b/2+i/4|B|-\varepsilon(b-2)/2)}.\tag{3.11b}$$

It can be shown that at b = 1 or 2 the coefficients $C_\pm$ do not depend on ϵ, with $C_+ = C_-^*$. Their absolute values are determined by the relations

$$|C_\pm(b,|B|)|^2=\frac{1-\exp(-\pi/2|B|)}{2\pi}(4|B|)^{b-1}\quad(b=1,2).\tag{3.12}$$

The scattering phase shift $\operatorname{Im}\ln C_0(1, |B|)$ as a function of $1/4|B|$ is shown in Fig. 3. As $B \to 0$, the $\operatorname{Im}\ln C_0(1, |B|)$ curve tends to $\pi/4$.

Direct calculation shows that the first nonvanishing term of the quasiclassical asymptotic form of the Green's function (3.11), together with the pre-exponential coefficient $C_+ = C_-^*$, yields, in the limit of large deformations $|B| \gg 1$, the correct result for the integrated intensity R_i of the scattered wave, equal to the corresponding

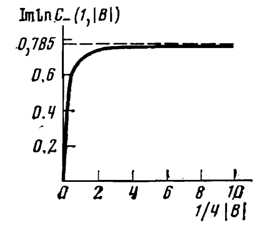

FIG. 3. Dependence of the scattering phase on the deformation.

value calculated by perturbation theory (the kinematic limit). The point is that now, in comparison with geometric optics[2], the expression for the intensity R_i contains the statistical scattering factor $|C_+|^2 = |C_-|^2 = 1 - \exp(-\pi/2|B|)$, which tends to zero as $|B| \to \infty$. Physically this is connected with the fact that as the deformation $|B|$ increases the volume of the scattering region of the crystal decreases like $1 - \exp(-\pi/2|B|)$.

As a rule, the case when the strain gradient is small is realized in a deformed crystal far from the stress concentrators. It is interesting that in this case it is possible to write down a general formula that approximates uniformly the Green's function with a fixed relative accuracy $\delta < 1$. Inasmuch as at $|B| \ll 1$ we have

$$\operatorname{Im}\ln C_-(b,|B|)\approx-\frac{\pi}{2}\left(b-\frac{1}{2}\right),$$

we obtain from (3.11) and (3.12)

$$\begin{gathered}{}_1F_1\left(1+i\frac{\sigma^2}{4B}, b; iB\rho^2\right)\sim\Gamma(b)\exp\left(\frac{iB\rho^2}{2}\right)\left(\frac{\rho}{2}\right)^{1-b}\\ \times(2\pi)^{-1/2}(\rho^2(1+b^2\rho^2))^{-1/4}\left\{\exp\left[iS(\rho)-i\pi\left(\frac{b-1}{2}+\frac{1}{4}\right)\right]\right.\\ \left.+\exp\left[-iS(\rho)+i\pi\left(\frac{b-1}{2}+\frac{1}{4}\right)\right]\right\}.\end{gathered}\tag{3.13}$$

It is easy to show that the regions of applicability of the expansions (3.9)–(3.13) at large $|\kappa|$ overlap, in which case

$$\begin{gathered}{}_1F_1\left(1+i\frac{\sigma^2}{4B}, b; iB\rho^2\right)\sim\Gamma(b)\exp\left(\frac{iB\rho^2}{2}\right)\left(\frac{\rho}{2}\right)^{1-b}\\ \times S(\rho)(\rho^2(1+B^2\rho^2))^{-1/4}J_{b-1}(S(\rho))(1+0(|B|^{1/2}))\end{gathered}\tag{3.14}$$

uniformly in the entire influence region $|x| \leq z$.

The interpolation formula (3.14) is similar to the corresponding expression for the Green's function in a perfect crystal.[5] Just as in a perfect crystal, the surfaces of the wave front of the perturbation propagating in the medium are hyperbolic cylinders with ρ = const, but the phase on the wave front $S(\rho)$ is now a complicated function of ρ (see (3.10)). It can be shown (for details see below) that the function $S(\rho)$ has the physical meaning of the phase integral along the ray trajectories, which are hyperbolas in a crystal with a strain gradient $|B| \ll 1$. Expressions (3.9)–(3.13) describe also the scattering of x rays in inhomogeneous crystals in a wide interval of values of the effective deformation parameter B, the absorption coefficient k, and the scattering asymmetry parameter β, under the condition that the strain gradient changes slowly over distances on the order of the crystal thickness.

4. THE EIKONAL APPROXIMATION

It is physically clear that the wave field in a crystal with a small strain gradient can be found by the trajectory method. The geometric-optics theory based on the trajectory approach, as applied to the problem of DXRS on a bent crystal, was considered in detail by Kato.[2]

We shall show that the results of the Kato theory follow directly from the asymptotic expansion of the influence function (3.13). With the aid of (3.10) and (2.9) we can write down an explicit expression for the eikonal

$$\begin{aligned}\Phi_\pm(\mathbf{r}_P,\mathbf{r})&=\eta(\mathbf{r}_P-\mathbf{r})+B\rho^2/2+S_0(\mathbf{r}_P,\mathbf{r})\pm S(\rho)\\&=\eta(\mathbf{r}_P-\mathbf{r})+B\rho^2/2+S_0(\mathbf{r}_P,\mathbf{r})\pm\rho\sqrt{1+B^2\rho^2}/2\\&\mp\frac{1+2ik}{2|B|}\ln(\sqrt{1+B^2\rho^2}-|B|\rho)\mp i\varepsilon(b-2)\ln(\sqrt{1+B^2\rho^2}-|B|\rho).\end{aligned}\qquad(4.1)$$

In (4.1), the third and fourth terms of the right-hand side coincide exactly with the complex eikonal of the Kato theory[2], with allowance for the transition formulas

$$Z=2Bz,\quad X=2Bx,\quad M=-kz,$$

where Z, X, and M are the Kato variables. The fifth term of (4.1) is included in the Kato theory in the amplitude of the scattered wave. The dependence of this term on the sign of the deformation leads to violation of the Firedel law for absorbing crystals, i.e., to a change of the integral intensity of the scattered wave when the direction of the strain gradient (or of the reflection vector **h**) is changed.

We consider now a wave packet incident on the surface of a bent crystal. The wave field inside and at the exit from the crystal is given by expressions (2.11) with the influence functions (2.9). If the spatial length of variation of the packet is large in comparison with the extinction length Λ, we can use the stationary phase method in the eikonal approximation for the calculation of the integrals (2.11). The stationary points at fixed coordinates of the observation point (x_P, z_P) are determined from the two equations for the weakly and strongly absorbed waves:

$$\frac{\partial}{\partial x}(\Phi_\pm'(x_P,x,z_P,0))=0,\qquad(4.2)$$

where the prime denotes the real part of the eikonal.

Equations (4.2) can be regarded as the equations for the ray trajectories emerging from two points on the entrance surface, with a common running observation point (x_P, z_P). Substituting in (4.2) the expression for the eikonal (4.1) we obtain after direct calculations

$$(2B(x_P-x)\mp\xi(x))^2-(2Bz_P-\eta(x))^2=1,\qquad(4.3)$$

where

$$\eta(x)=\eta_x'+(C-B)x,\quad \xi(x)=(1+\eta^2(x))^{1/2}.\qquad(4.4)$$

Here $\eta(x)$ determines the deviation from the exact Bragg condition at the point x on the entrance surface of the crystal.

It is seen from (4.3) that the trajectories of the rays constitute a family of hyperbolas, and that physical meaning attaches to the hyperbola branches satisfying the condition $|x_P - x| < z_P$. In the general case the hyperbolas form a "fan" that can be either converging or diverging, depending on the branch of the dispersion surface (weakly and strongly absorbed waves) and on the sign of the deformation. In principle, the formation of caustics is possible here, i.e., the formation of points of intersections of the rays, where the geometric-optics theory does not hold. The positions of the caustics are determined (see, e.g.,[19]) by simultaneous solution of two equations, the first of which is (4.2) and the second is

$$\frac{\partial^2}{\partial x^2}[\Phi_\pm'(x_P,x,z_P,0)]=0\qquad(4.5a)$$

or, equivalently, if we know the solution of the equations for the trajectories $x_P = x_P(z_P, x, 0)$,

$$dx_P/dx=0.\qquad(4.5b)$$

By way of example we consider the symmetric scattering of x rays by a bent crystal ($B = 0$, $C \neq 0$) in the case of an incident plane wave. At $B = 0$ the ray trajectories form two families of straight lines (cf. (4.3))

$$x_P-x=\pm\frac{\eta(x)}{\xi(x)}z_P.\qquad(4.6)$$

Combining (4.5b) and (4.6) we find that at $C > 0$ (< 0) the rays corresponding to the strongly (weakly) absorbed wave form a caustic, the equation of which is

$$(Cx_P+\eta_x')^2=[(Cz_P)^{2/3}-1]^3.\qquad(4.7)$$

It follows from (4.7) that the critical thickness of the crystal, starting with which ray focusing takes place, is equal to

$$|C|z_P=1\text{ and }Cx_P+\eta_x'=0.\qquad(4.8)$$

The intersection of the caustic surface with the scattering plane is shown graphically in Fig. 4. The caustic divides the scattering plane into two regions. In the upper region, far from the caustic, we can use the stationary-phase method to find the field of the scattered wave, which forms on emerging from the crystal an approximately converging beam of x rays.[10]

Thus, on the basis of an exact solution of the DXRS problem in a crystal with a constant strain gradient it is possible to construct a quasiclassical asymptotic expression for the wave field, to calculate the pre-exponential coefficient in a wide range of values of the scattering parameters, and establish the limits of applicability of the trajectory approach of the geometric-optics theory. At the same time, the use of the quasiclassical asymptotic form of the Green's function makes it possible to reveal directly the physically significant features of the DXRS in an elastically bent crystal, particularly the formation of a caustic, and to calculate in principle the structure of the wave field both far from and close to the caustic.

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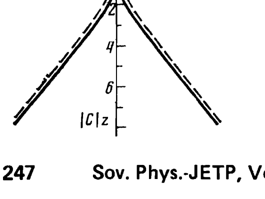

FIG. 4. Intersection of the caustic surface and the scattering plane.

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