Diffractive x-ray focusing upon Bragg reflection by biaxially curved perfect cyrstal

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A theory is derived for $2D$ diffractive focusing of x-rays upon Bragg reflection from an elastically curved perfect crystal. The general problem of the diffraction of a spherical wave emitted by a point source is analyzed in the geometry of asymmetric reflection with an arbitrary source-to-crystal distance. Equations are derived for the imaging of x-ray beams by means of a biaxially curved crystal, used as a diffractive lens. In the case of symmetric Bragg reflection, and for a certain relation between the radii of curvature, specifically, $R_y = R_x \sin^2\vartheta$ (R_x and R_y are the radii of curvature in the sagittal and meridional planes, respectively, and ϑ is the Bragg angle), a lens of this sort images homocentric x-ray beams without astigmatism in accordance with the formula $L_0^{-1} + L_h^{-1} = F^{-1}$, where $F = (1/2)R_x \sin\vartheta$ is the focal length, L is the distance from the source to the crystal, and L_h is the distance from the crystal to the image. Equations are derived for the spectral and spatial aberrations of an x-ray lens. The diffractive broadening of the focus is found, as is the blurring of the focus which results from the nonzero angular divergence and nonmonochromatic nature of the incident radiation. Theoretical estimates of the focus size in the case of $2D$ focusing of x rays upon Bragg back reflection agree in order of magnitude with an experimental value found by Kushnir and Suvorov [JETP Lett. **48**, 117 (1988)].

Experiments with x rays ordinarily use radiation wavelengths $\lambda \sim 1$–100 Å, and the spectral and angular resolution required can be varied over six orders of magnitude, from $\Delta\lambda/\lambda$, $\Delta\vartheta \sim 10^{-1}$ for small-angle scattering and fluorescence analysis to $\Delta\lambda/\lambda \sim 10^{-7}$ in x-ray spectroscopy and $\Delta\vartheta \sim 10^{-7}$ in three-crystal diffractometry. In recent years, particularly because of the promising outlook for the widespread use of intense sources of synchrotron radiation,[1] there has been a rapid development of x-ray optics based on focusing monochromators-collimators, for producing beams with given spectral and angular characteristics. While for soft x radiation ($\lambda \sim 20$–100 Å) there already exist focusing elements such as Fresnel zone plates and curved mirrors, which operate at grazing angles of incidence, and there are even x-ray microscopes with a resolution ~ 500 Å (Ref. 2, for example), in the case of hard radiation, with $\lambda \sim 1$ Å, the development of similar x-ray-optics focusing devices remains an open question.

There are various methods available for cylindrical ($1D$) focusing of x rays, by means of plane and uniaxially curved diffracting crystals. In this case, the radiation is collected to a line oriented perpendicular to the plane of diffractive scattering. A comprehensive bibliography of the theoretical and experimental work on $1D$ focusing is given in the reviews by Chukhovskiĭ[3,4] (see also Ref. 1). Clearly, however, the case of greatest interest is that of spherical ($2D$) focusing of x radiation, in which a point focus is formed. This possibility has been discussed in principle in theoretical papers[5–8] on the basis of geometric-optics representations. It was shown by Berreman *et al.*,[5] for example, that a $2D$ focusing can be achieved in a generalized Johann-Hamos arrangement with the help of a biaxially curved crystal if the radii of curvature in the two mutually perpendicular planes satisfy a certain relation. Kushnir *et al.*[6] proposed a method for focusing by means of a biaxially curved crystal under conditions of three-ways diffraction, but they showed that this arrangement requires an angular collimation of the order of 10^{-5} in two planes and therefore has a low luminosity. Levonyan and Balyan[7] have pointed out the possibility of a $2D$ focusing upon symmetric Laue diffraction by a perfect crystal curved around an axis passing through the points which are the positions of the source and the focus. Gabrielyan[8] and Kushnir and Suvorov[9] have recently reported a (plane wave)-to-point focusing a x radiation upon Bragg reflection from a biaxially curved crystal. Kushnir and Suvorov[9] experimentally achieved a $2D$ focusing in the backscattering of Co $K\alpha_1$ radiation from a spherically curved Ge crystal (mirror).

In the present paper we take up a dynamic theory of $2D$ focusing of x radiation in the general case of an asymmetric Bragg-diffraction geometry, with an arbitrary distance from the source to the biaxially curved crystal. We work from the exact solution of the problem of the dynamic diffraction of x rays in the case of a uniaxially curved crystal,[10] and we use the method of point-source functions[11] to find the field distribution of the diffracted wave in vacuum. We find the focusing conditions, the geometric characteristics of the focusing, the dimensions of the diffractive broadening of a point focus, and the broadening of this focus due to the nonzero dimensions (linear or angular) of the radiation source.

1. DERIVATION OF BASIC RELATIONS

A monochromatic packet of x radiation $\mathbf{E}_0(\mathbf{r}, t) = \widetilde{\mathbf{E}}(\mathbf{r}, \omega)\exp(i\mathbf{k}_0\mathbf{r} - i\omega t)$ is incident on a biaxially curved crystal (Fig. 1) which is oriented in such a way that two-wave Bragg diffraction occurs in the initial state, with radii of curvature R_x, $R_y \to \infty$. The wave field in the crystal is a coherent superposition of the transmitted and Bragg-reflected waves:

$$\mathbf{E}(\mathbf{r}, t) = \{\mathbf{e}_0 E_0(\mathbf{r}, \omega)\exp(i\mathbf{k}_0\mathbf{r}) + \mathbf{e}_h E_h(\mathbf{r}, \omega)\exp(i\mathbf{k}_h\mathbf{r})\}\cdot\exp(-i\omega t), \quad (1)$$

where the wave vectors $\mathbf{k}_0$ and $\mathbf{k}_h$ are related by the Bragg relation $\mathbf{k}_h = \mathbf{k}_0 + \mathbf{h}$; $\mathbf{e}_0$, $\mathbf{e}_h$ are unit polarization vectors; and $\mathbf{h}$ is a reciprocal-lattice vector of the perfect crystal, multiplied by 2π.

Substituting (1) into Maxwell's equation

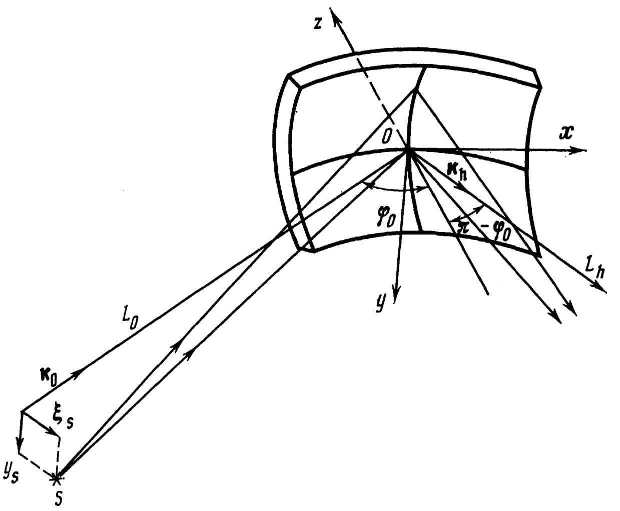

FIG. 1. Geometry of the Bragg scattering of x radiation emitted by point source S, which lies at a distance L_0 from a biaxially curved single-crystal plate.

$$\mathrm{rot\,rot}\,\mathbf{E}(\mathbf{r},\omega)=\varkappa^2\varepsilon(\mathbf{r},\omega)\mathbf{E}(\mathbf{r},\omega),\quad \varkappa=\omega/c,$$

which describes the propagation of the wave field in a deformed crystal with a dielectric constant

$$\varepsilon(\mathbf{r},\omega)=1+\sum_{\mathbf{h}}\chi_h\exp[i\mathbf{hr}-i\mathbf{hu}(\mathbf{r})],$$

where χ_h are Fourier components of the polarizability of the perfect crystal, and $\mathbf{u}(\mathbf{r})$ is the vector elastic displacement of the atoms of the crystal lattice, we find the following system of equations, which relates the amplitudes E_0 and E_h (Ref. 12, for example):

$$\begin{aligned}&\mathrm{rot\,rot}(\mathbf{e}_0E_0)+2i(\mathbf{k}_0\,\mathrm{grad})(\mathbf{e}_0E_0)\\&+\varkappa^2\chi_0\mathbf{e}_0E_0+\varkappa^2\chi_{-h}\exp(i\mathbf{hu})\mathbf{e}_hE_h=0,\\&\mathrm{rot\,rot}(\mathbf{e}_hE_h)+2i(\mathbf{k}_h\,\mathrm{grad})(\mathbf{e}_hE_h)\\&+\varkappa^2\chi_0\mathbf{e}_hE_h+\varkappa^2\chi_h\exp(-i\mathbf{hu})\mathbf{e}_0E_0=0.\end{aligned}\tag{2}$$

The derivation of (2) made use of the circumstance that under the conditions of this problem the transmitted wave and the diffracted wave can be assumed to be strictly transverse, i.e., $\mathbf{e}_0\mathbf{k}_0=\mathbf{e}_h\mathbf{k}_h=0$.

In the case of elastic curvature of a thin single-crystal plate with radii of curvature R_x and R_y (Fig. 2), the general solution of the equations of the anisotropic theory of elasticity leads to the following expression for the displacement vector $\mathbf{u}(\mathbf{r})$ (Ref. 13):

$$\begin{aligned}u_x&=\frac{x}{R_x}\left(z-\frac{t}{2}\right)-\frac{1}{2}\left(\frac{A_{11}}{R_x}-\frac{A_{12}}{R_y}\right)\left(z-\frac{t}{2}\right)^2,\\u_y&=\frac{y}{R_y}\left(z-\frac{t}{2}\right)-\frac{1}{2}\left(\frac{A_{21}}{R_x}-\frac{A_{22}}{R_y}\right)\left(z-\frac{t}{2}\right)^2,\\u_z&=-\frac{x^2}{2R_x}-\frac{y^2}{2R_y}-\frac{1}{2}\left(\frac{A_{31}}{R_x}-\frac{A_{32}}{R_y}\right)\left(z-\frac{t}{2}\right)^2,\end{aligned}\tag{3}$$

where the coefficients A_{ij} are certain combinations of the components of the reciprocal of the elastic-modulus tensor a_{ik}, and t is the thickness of the crystal plate.

In the scattering geometry assumed here (Fig. 1), the function describing the displacement of the reflecting planes, $\mathbf{h}\cdot\mathbf{u}(\mathbf{r})$, in (2) takes the following form when we make use of (3):

$$\mathbf{hu}(\mathbf{r})=\mathbf{h}\tilde{\mathbf{u}}(x,z)+\varkappa(\gamma_0-\gamma_h)y^2/2R_y,\quad \gamma_{0,h}=\cos\varphi_{0,h}.\tag{4}$$

Here we have introduced the simplified function

$$\begin{aligned}\mathbf{hu}(x,z)=\varkappa(\sin\varphi_h-\sin\varphi_0)&\left[\frac{x}{R_x}\left(z-\frac{t}{2}\right)\right.\\&\left.-\frac{1}{2}\left(\frac{A_{11}}{R_x}-\frac{A_{12}}{R_y}\right)\left(z-\frac{t}{2}\right)^2\right]\\&+\varkappa(\gamma_h-\gamma_0)\left[-\frac{x^2}{2R_x}-\frac{1}{2}\left(\frac{A_{31}}{R_x}-\frac{A_{32}}{R_y}\right)\left(z-\frac{t}{2}\right)^2\right].\end{aligned}\tag{5}$$

In writing (4) and (5) we omitted terms which are linear in the coordinates x, y, z; such terms are known (Ref. 10, for example) to lead to only a renormalization of the exact Bragg angle.

Under the assumption that on the crystal surface $x=0$ the linear dimensions $x_{\rm eff}$ and $y_{\rm eff}$ of the region of effective diffractive scattering are much smaller than the distance L_0, from the source to the crystal we find for the amplitude $\tilde{E}(\mathbf{r},w)$ of the incident wave the following expression which holds within terms in the phase which are quadratic in the coordinates x, y, inclusively (this is the parabolic approximation, $z=0$):

$$\begin{aligned}&\mathrm{Im}\ln\tilde{E}(x,y,0)\\&=\varkappa\left[L_0+\frac{1}{2L_0}(x\cos\varphi_0-\xi_S)^2+\frac{1}{2L_0}(y-y_S)^2\right],\end{aligned}\tag{6}$$

where ξ_S, Y_S are the coordinates of point source S (Fig. 1).

The diffractive scattering of x-ray waves in crystal is generally described by the system of dynamic second-order partial differential equations (2). In the case at hand, these equations can be simplified since it is clear from physical considerations that the low strength of the interaction of the x rays with the crystal, characterized by the quantity $|\chi_h|\sim10^{-5}$, will cause the characteristic distances for the variations in the amplitudes E_0 and E_h of the wave field to be much larger than the wavelength of the radiation, $\lambda\sim1$ Å. This circumstance means that we can ignore the second derivatives $\partial^2/\partial x^2$, $\partial^2/\partial z^2$ in (2) in comparison with the first derivatives. We also assume

$$|\partial^2E_{0,h}/\partial y^2|\ll\varkappa^2|\chi_h||E_{0,h}|.\tag{7}$$

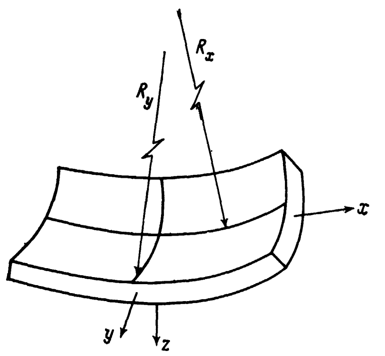

FIG. 2. Biaxial curvature of the crystalline plate. R_x and R_y are the radii of curvature in respectively the sagittal and meridional planes of the Bragg scattering.

Writing the unknown amplitudes of the wave field in the form [see (4)–(6)]

$$E_0(\mathbf{r})=\mathscr{E}_0(x,z)\exp\left[\frac{i\varkappa(y-y_s)^2}{2L_0}\right],$$
$$E_h(\mathbf{r})=\mathscr{E}_h(x,z)\exp\left[\frac{i\varkappa(y-y_s)^2}{2L_0}-\frac{i\varkappa(\gamma_0-\gamma_h)y^2}{2R_y}\right], \qquad (8)$$

we find from (2) the following system of first-order partial differential equations:

$$i\sin\varphi_0\frac{\partial\mathscr{E}_0}{\partial x}+i\gamma_0\frac{\partial\mathscr{E}_0}{\partial z}+\frac{\varkappa\chi_0}{2}\mathscr{E}_0+\frac{\varkappa\mathscr{C}\chi_{-h}}{2}\exp(i\mathbf{h}\tilde{\mathbf{u}})\mathscr{E}_h=0,$$
$$i\sin\varphi_h\frac{\partial\mathscr{E}_h}{\partial x}+i\gamma_h\frac{\partial\mathscr{E}_h}{\partial z}+\frac{\varkappa\chi_0}{2}\mathscr{E}_h+\frac{\varkappa\mathscr{C}\chi_h}{2}\exp(-i\mathbf{h}\tilde{\mathbf{u}})\mathscr{E}_0=0. \qquad (9)$$

These equations are to be used to determine the amplitudes $\mathscr{E}_0$, $\mathscr{E}_h$, where $\mathscr{C}$ is a polarization factor, which has the value $\mathscr{C}=1$ for σ-polarized radiation and $\mathscr{C}=\cos 2\vartheta$ for π-polarized radiation.

When the explicit dependence of amplitudes (8) on the coordinate y is taken into account, condition (7) imposes the restriction

$$y_{eff}\lesssim|\chi_h^{1/2}R_y|$$

on the linear dimension of the diffraction region, for which we can carry out a systematic analysis on the basis of Eqs. (9).

The problem of the Bragg scattering of x rays in a biaxially curved crystal is thereby reduced to the problem of solving equations (9), which are dynamic equations of cylindrical x-ray optics with displacement-field function (5). An exact solution of the boundary-value problem of the Bragg diffraction of x rays in an elastically curved crystal leads to the following expression for the amplitude $\mathscr{E}_h$ at the surface $z=0$ of a semi-infinite crystal (Ref. 10):

$$\mathscr{E}_h(x,0)=\frac{i\varkappa\mathscr{C}\chi_h}{4a|\gamma_h|}\exp\left(\frac{i\varkappa\gamma_h}{2R_x}x^2\right)\int_{-\infty}^{\infty}dx'\,G_{h0}(x-x')\tilde{\mathscr{E}}(x',0)$$
$$\times\exp\left[-\frac{i\varkappa\gamma_0^2}{2R_x}x'^2+iq_0(x-x')\right]. \qquad (10)$$

This expression for the amplitude is written in terms of the Green's function

$$G_{h0}(x)=\frac{1}{2\pi i}\int_{p_0-i\infty}^{p_0+i\infty}dp\,G_h(p)e^{px}, \qquad (11)$$

where the Laplace transform $G_h(p)$ is

$$G_h(p)=\left(\frac{i}{4B}\right)^{1/2}D_{-1-\nu}\left[i\left(\frac{i}{4B}\right)^{1/2}p\right]\Big/D_{-\nu}\left[i\left(\frac{i}{4B}\right)^{1/2}p\right]. \qquad (11')$$

Here we are using the notation

$$q_0=\frac{\varkappa\chi_0}{4a}\left(\frac{1}{\gamma_0}-\frac{1}{\gamma_h}\right),\qquad 2a=a_0-a_h,\qquad a_{0,h}=\mathrm{tg}\,\varphi_{0,h},$$
$$\nu=i\frac{\varkappa^2\mathscr{C}^2\gamma_0|\gamma_h|\chi_h\chi_{-h}}{16B\sin^2 2\vartheta},\qquad B=\frac{1}{4}\frac{\partial^2(\mathbf{h}\tilde{\mathbf{u}}(x,z))}{\partial(x-a_0z)\,\partial(x-a_hz)}, \qquad (12)$$

where $D_\nu(t)$ is the parabolic cylinder function.

Substituting (6) and (11) into (10), and using (8), we find the following expression for the amplitude of the diffracted radiation at the front face of the crystal, after direct calculations:

$$E_h(x,y,0)=\frac{2^{1/2}\varkappa^{1/2}\mathscr{C}\chi_h}{16\pi^{1/2}aL_0\alpha_0^{1/2}|\gamma_h|}\exp\left\{i\left[\frac{3\pi}{4}+\varkappa L_0-\frac{\varkappa(\gamma_0-\gamma_h)}{2R_y}y^2+\frac{\varkappa}{2L_0}(y-y_s)^2-\frac{\varkappa\gamma_h}{2R_x}x^2-\frac{\varkappa\xi_s^2}{2L_0}\right]\right\}$$
$$\times\frac{1}{2\pi}\int dk\,G_h(k+q_0)\exp[i\mathscr{F}(k,x)]. \qquad (13)$$

Here the eikonal function $\mathscr{F}(k,x)$ is

$$\mathscr{F}(k,x)=-k^2/2\varkappa\alpha_0-k(x-\gamma_0\xi_s/\alpha_0L_0), \qquad (14)$$

where $\alpha_0=\gamma_0^2/L_0-\gamma_0/R_x$.

For simplicity we will restrict the discussion below to the case of only a slight curvature of the reflecting planes of the crystal, in which we have $|\nu|\gg 1$ or, in expanded form, a dimensionless curvature parameter

$$\frac{\varkappa\Lambda^2}{4\pi^2}\left|\frac{a_0\sin\varphi_0-a_h\sin\varphi_h}{R_x}\right|\ll 1, \qquad (15)$$

where the x-ray extinction length in the perfect crystal is

$$\Lambda=\lambda|\gamma_0\gamma_h|^{1/2}/\mathscr{C}|\chi_h\chi_{-h}|^{1/2}.$$

In this case the Fourier component of the Green's function [see (11')] takes the form of the corresponding expression for a perfect crystal:

$$G_h(k)=2i[k+(k^2-\pi^2/a^2\Lambda^2)^{1/2}]^{-1}. \qquad (16)$$

2. DIFFRACTED WAVE IN VACUUM

To find the distribution of the diffracted radiation which escapes through the upper face of the crystal into vacuum, we would generally have to apply a direct Fourier transformation to (13) and then, taking into account the joining of each plane-wave harmonic, take the inverse transformation, working from the standard condition of the continuity of the tangential components of the wave vectors. A simpler procedure, which leads to the same result, is to use the Huygens-Fresnel principle from optics, according to which the diffracted wave in vacuum at the point $\mathbf{r}_p$ is written as the convolution of the diffracted wave of the surface of the crystal, (13), with a point-source function (Green's function) in vacuum[11]:

$$E_h(\mathbf{r}_P)\exp(i\mathbf{k}_h\mathbf{r}_P)$$
$$=2i\gamma_h\iint dy\,dx\,E_h(x,y,0)\exp(i\mathbf{k}_h\mathbf{r})G_0(|\mathbf{r}_P-\mathbf{r}|), \qquad (17)$$

where

$$G_0(r)=(4\pi r)^{-1}\exp(i\varkappa r).$$

As was shown above for the case of an incident spherical wave [see (6)], the phase of the Green's function $G_0(|\mathbf{r}_p-\mathbf{r}|)$ in (17) can be expanded in powers of x^2/L_h^2, $y^2/L_h^2\ll 1$. Correspondingly, restricting the analysis to the parabolic approximation, we have

$$\mathrm{Im}\ln G_0(|\mathbf{r}_P-\mathbf{r}|)$$
$$=\varkappa[L_h-x\sin\varphi_h+(\xi_P+x\gamma_h)^2/2L_h+(y_P-y)^2/2L_h]. \qquad (18)$$

Substituting (13), (14), and (18) into (17), and carrying out some simple calculations (which we will not reproduce here), we find the following expression for the diffracted wave in vacuum (which holds within an inconsequential phase factor):

$$E_h(\mathbf{r}_P)=\frac{\varkappa\mathscr{C}\chi_h}{16\pi a L_0 L_h}(\alpha_0\alpha_h)^{-1/2}$$
$$\times\frac{1}{2\pi}\int dy\int dk\, G_h(k+q_0)\exp[i\mathscr{F}_{sph}(k,y)], \qquad (19)$$

where the eikonal function $\mathscr{F}_{\rm sph}(k,y)$ is

$$\mathscr{F}_{sph}(k,y)=-\frac{k^2}{2\varkappa}\left(\frac{1}{\alpha_0}+\frac{1}{\alpha_h}\right)+k\left(\frac{\gamma_0\xi_S}{\alpha_0 L_0}+\frac{\gamma_h\xi_P}{\alpha_h L_h}\right)$$
$$+\frac{\varkappa y^2}{2}\left(\frac{1}{L_0}+\frac{1}{L_h}-\frac{\gamma_0-\gamma_h}{R_y}\right)-\varkappa y\left(\frac{y_P}{L_h}+\frac{y_S}{L_0}\right). \qquad (20)$$

The parameters α_0 and α_h determine the geometry of the diffractive reflection. Specifically, α_h is related to the radius of curvature R_x and to the distance L_h by (cf. α_0)

$$\alpha_h=\gamma_h^2/L_h+\gamma_h/R_x. \qquad (21)$$

A case of practical interest is that of an incident plane wave, in which we would have $L_0\gg\gamma_0|R_x|$. Taking the limit $L_0\to\infty$ in (20), we easily find that in the Bragg reflection of a monochromatic plane wave from a biaxially curved crystal the diffracted wave is described by [see (19)]

$$E_h(\mathbf{r}_P)=\frac{\varkappa\mathscr{C}\chi_h}{4aL_h}\left(\frac{\gamma_0\alpha_h}{R_x}\right)^{-1/2}$$
$$\times\frac{1}{2\pi}\int dy\int dk\, G_h(k+q_0)\exp[i\mathscr{F}_{pl}(k,y)], \qquad (22)$$

where the eikonal function $\mathscr{F}_{pl}(k,y)$ is [cf. (20)]

$$\mathscr{F}_{pl}(k,y)=-\frac{k^2}{2\varkappa}\left(-\frac{R_x}{\gamma_0}+\frac{1}{\alpha_h}\right)+k\left(R_x\Delta\varphi_\xi+\frac{\gamma_h\xi_P}{\alpha_h L_h}\right)$$
$$+\frac{\varkappa y^2}{2}\left(\frac{1}{L_h}-\frac{\gamma_0-\gamma_h}{R_y}\right)-\varkappa y\left(\frac{y_P}{L_h}+\Delta\varphi_y\right), \qquad (23)$$

where $\Delta\varphi_\xi$ and $\Delta\varphi_y$ give the angular deviations of the incident plane wave from the exact Bragg direction in respectively the sagittal and meridional planes.

Expressions (19)–(23) can be used to calculate the spatial distribution of the diffracted radiation in vacuum under very general assumptions regarding the geometry of the Bragg reflection, for arbitrary radii of curvature of the crystal. From the physical standpoint, the Bragg-reflection arrangements of greatest interest are those in which the curved diffracting crystal operates as a spherical x-ray lens which focuses x-ray beams "point-to-point" or "point-to-(parallel beam)."

3. JOHANN-HAMOS FOCUSING SPECTROMETER

Before we analyze the arrangements listed above, we wish to discuss Johann-Hamos focusing, in which a point source of radiation is in the sagittal plane ($y=0$) on the Rowland circle, whose diameter is equal to the crystal radius of curvature R_x ($\alpha_0=0$); this corresponds to the following distance from the source of the crystal (Fig. 3)[14,15]:

$$L_0^{(*)}=\gamma_0 R_x. \qquad (24)$$

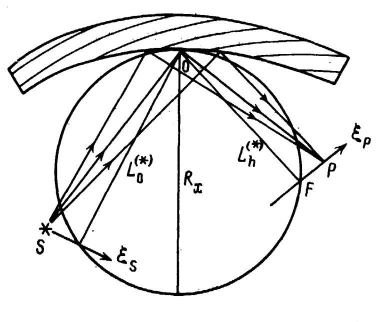

FIG. 3. Diagram used in the discussion of a focusing Johann-Hamos spectrometer. Ray paths in the sagittal plane.

In the limit $\alpha_0\to 0$ the function

$$(i/2\pi\varkappa\alpha_0)^{1/2}\exp(-ik^2/2\varkappa\alpha_0)$$

in the integrand in (19) reduces to a δ-function, and the integral in (19) can be evaluated immediately. As a result we find

$$E_h(\mathbf{r}_P)\propto\frac{\varkappa^{3/2}\mathscr{C}\chi_h}{16\pi a L_0^{(*)}L_h}(2\pi\alpha_h)^{-1/2}G_h\left(q_0+\frac{\varkappa\xi_S}{R_x}\right)\int dy\exp\left[i\frac{\varkappa y^2}{2}\left(\frac{1}{L_0^{(*)}}+\frac{1}{L_h}-\frac{\gamma_0-\gamma_h}{R_y}\right)-i\varkappa y\left(\frac{y_P}{L_h}+\frac{y_S}{L_0^{(*)}}\right)\right]. \qquad (25)$$

In other words, the amplitude of the diffracted wave in vacuum is directly proportional to the Fourier component of the Green's function, $G_h(q_0+\varkappa\xi s/R_x)$. It can also be seen from (25) that $E_h(\mathbf{r}_p)$ becomes infinite at a point whose coordinate L_h is determined by the condition $\alpha_h=0$. The explicit expression for this coordinate is

$$L_h^{(*)}=|\gamma_h|R_x. \qquad (26)$$

Clearly, however, the divergence of $E_h(\mathbf{r}_p)$ as $\alpha_h\to 0$ is nonphysical; it is a consequence of the approximations used in deriving (25), in particular, expansions (6) and (18). Actually, we need to take into account the circumstance that the diffracted radiation is collected from a finite length of diffractive reflection along the surface of the crystal, $x_{\rm eff}$, which is limited in turn by the distance at which the geometric aberration of the reflected x-ray beams starts to be important.[11]

It is not difficult to show that when the finite diffractive-reflection length $x_{\rm eff}$ is taken into account direct calculations based on Eqs. (13), (17), (24), and (26) lead to the following expression for the intensity distribution of the diffracted radiation near the point L_h^* [cf. expression (17) in Ref. 11]:

$$I_h(\mathbf{r}_P)=|E_h(\mathbf{r}_P)|^2\propto\left|\frac{\varkappa^2\mathscr{C}\chi_h}{16\pi^2R_x^2\sin^2 2\vartheta}\right.$$
$$\times G_h\left(q_0+\frac{\varkappa\xi_S}{R_x}\right)\frac{\sin[\varkappa x_{eff}(\xi_P+\xi_S)/2R_x]}{\varkappa(\xi_P+\xi_S)/2R_x}$$
$$\times\int dy\exp\left\{i\frac{\varkappa y^2}{2R_x}\left[\frac{1}{\gamma_0}-\frac{1}{\gamma_h}-\frac{R_x}{R_y}(\gamma_0-\gamma_h)\right]\right.$$
$$\left.\left.-i\frac{\varkappa y}{R_x}\left(\frac{y_P}{|\gamma_h|}+\frac{y_S}{\gamma_0}\right)\right\}\right|^2. \qquad (27)$$

It follows from (27) that under the relation

$$R_y=R_x\gamma_0|\gamma_h| \tag{28}$$

between the radii of curvature of the crystal the diffracted beam is focused at the point $\mathbf{r}_p^{(*)}$, with the Cartesian coordinates

$$\mathbf{r}_P^{(*)}=(\gamma_h\xi_S,\ (\gamma_h/\gamma_0)\,y_S,\ -\gamma_h^2R_x). \tag{29}$$

Relation (28) is a generalization of the Hamos condition for vertical focusing to the case of an asymmetric Bragg reflection of x rays from a biaxially curved crystal.

Intensity distribution (27) in the focal plane, $\xi_p y_p$, which is oriented perpendicular to the propagation direction of the diffracted wave in Fig. 3 (OF), has an absolute maximum at point (29), whose linear dimensions are, respectively,

$$\Delta\xi_P=\lambda R_x/x_{eff},\quad \Delta y_P=|\gamma_h|\lambda R_x/y_{eff}. \tag{30}$$

It also follows from (27) that from a spherical wave incident on a crystal under the condition $|\xi s|<\gamma_0R_x\delta$, where $\delta=\lambda/a\Lambda\gamma_0$ is the angular width of the Bragg reflection from a perfect crystal [see (16)], the part of the radiation in the solid angle $\delta\varphi_\xi\delta\varphi_y\sim x_{\rm eff}y_{\rm eff}/\gamma_0R_x^{\;2}$ is collected at the focusing point, (29).

We now wish to determine the linear dispersion $d\xi_p/d\lambda$ and the associated spectral resolution $d\lambda/\lambda$ of a Johann-Hamos focusing spectrometer. Since a change in the wavelength of the radiation leads to a change in the Bragg angle, $d\vartheta=(d\lambda/\lambda)\mathrm{tg}\,\vartheta$, we find from simple geometric considerations that the dispersion is

$$d\xi_P/d\lambda=(\gamma_0+\gamma_h)\,(R_x/\lambda)\,\mathrm{tg}\,\vartheta.$$

Using the first of equalities (30), we find an estimate of the spectral resolution:

$$d\lambda/\lambda=(\gamma_0+\gamma_h)^{-1}(\lambda/x_{eff})\,\mathrm{ctg}\,\vartheta. \tag{31}$$

The total range of wavelengths reflected by a diffracting crystal is $\Delta\lambda=\lambda\delta\cot\vartheta$. For the asymmetric 444 reflection of Mo $K\alpha$ radiation ($\lambda=0.7$ Å) from a Si single crystal ($\vartheta=26.9°$) with $R_x=10\,m$, $x_{\rm eff}=1$ cm, and $y_{\rm eff}=0.1$ cm, for example, estimates based on (30) and (31) yield the following values for the dimensions of the focus: $\Delta\xi_p\sim10^{-1}$ μm, $\Delta y_p\sim10^{-2}$ μm. The theoretical limit on the spectral resolution is $d\lambda/\lambda\sim10^{-8}$.

Strictly speaking, the results derived above apply to the case in which the size of the x-ray source, on the Rowland circle, satisfies the condition $\Delta\xi_s<\gamma_0R_x\delta$. In the opposite case $\Delta\xi_s>\gamma_0R_x\delta$, allowance for the nonzero dimensions of the source leads to the following expressions for the linear dispersion and the spectral resolution[11]:

$$\frac{d\xi_P}{d\lambda}=|\gamma_h|\frac{R_x}{\lambda}\,\mathrm{tg}\,\vartheta,\qquad \frac{d\lambda}{\lambda}=\frac{1}{|\gamma_h|}\left(\frac{\lambda}{x_{eff}}+\gamma_0\delta\right)\mathrm{ctg}\,\vartheta.$$

The total range of radiation wavelengths reflected from the crystal is $\Delta\lambda(\Delta\xi_s/\gamma_0R_x)\mathrm{ctg}\,\vartheta$.

4. POINT-TO-POINT FOCUSING; GENERAL CASE

In the general case, for an arbitrary distance from the source to the crystal, the Bragg reflection of a homocentric beam of x rays can be analyzed on the basis of Eqs. (19) and (20) by the stationary-phase method. The equations

$$\partial\mathcal{F}_{sph}(k,y)/\partial k=0,\quad \partial\mathcal{F}_{sph}(k,y)/\partial y=0 \tag{32}$$

determine the spatial fan of rectilinear ray trajectories which emerge from the front face of the crystal and which depend on the two parameters k and y. In turn, the relationship between the parameter k and the x coordinate of the point on the crystal surface ($z=0$) at which the ray emerges is determined by the stationary-phase equation of the integrand in (13):

$$k/\varkappa\alpha_0+x-\gamma_0\xi_S/\alpha_0L_0=0. \tag{33}$$

Combining (32) and (33), and going through some simple transformations, we find explicit equations for the ray trajectories:

$$\gamma_h\xi_P/\alpha_hL_h+\gamma_0\xi_S/\alpha_0L_0=-(1+\alpha_0/\alpha_h)\,(x-\gamma_0\xi_S/\alpha_0L_0),$$
$$y_P/L_h+y_S/L_0=y[1/L_0+1/L_h-(\gamma_0-\gamma_h)/R_y]. \tag{34}$$

As the radiation propagates through vacuum, different ray trajectories intersect, at generally different points whose positions are determined by the equations

$$\partial^2\mathcal{F}_{sph}(k,y)/\partial k^2=0,\quad \partial^2\mathcal{F}_{sph}(k,y)/\partial y^2=0. \tag{35}$$

These equations are none other than the equations of the imaging of a homocentric beam by a curved diffracting crystal. Explicitly, these equations are

$$\gamma_h^2/L_h+\gamma_0^2/L_0=(\gamma_0-\gamma_h)/R_x \tag{36}$$

in the sagittal plane and

$$1/L_h-1/L_0=(\gamma_0-\gamma_h)/R_y \tag{37}$$

in the meridional plane.

In the general case of the Bragg reflection of a homocentric beam by a biaxially curved crystal, the diffracted radiation is therefore an astigmatic beam with two focal lines. The distance between these lines depends on all of the following: the asymmetry of the diffraction geometry, the relation between the radii of curvature of the crystal, and the distance from the source of the crystal (Fig. 4).

There is, however, an imaging case of practical importance in which the homocentricity of beams is preserved in the course of Bragg reflection from a biaxially curved crystal. In the case of symmetric diffraction, with $\gamma_0=|\gamma_h|=\sin\vartheta$, and also when the relation

$$R_y=R_x\sin^2\vartheta \tag{38}$$

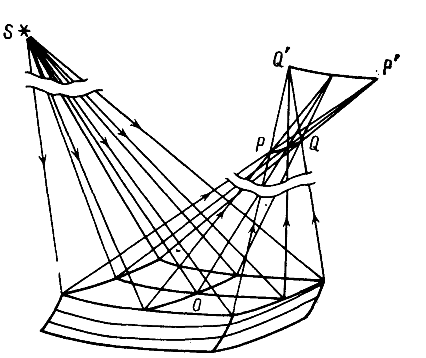

FIG. 4. Diagram used in analyzing point-to-point focusing accompanied by the formation of an astigmatic beam of diffracted radiation.

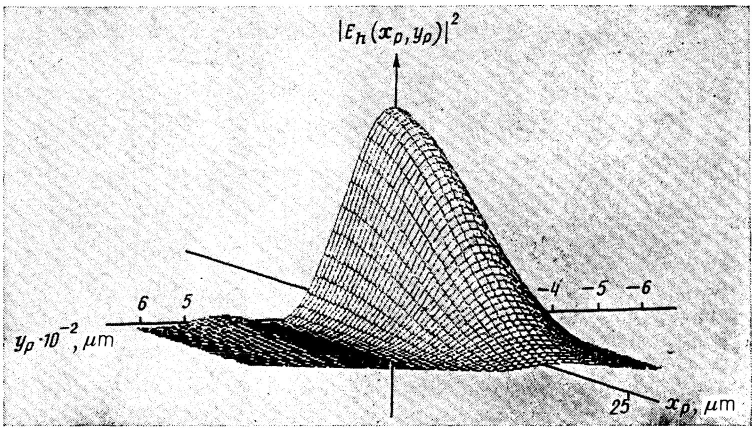

FIG. 5. Intensity distribution of the diffracted radiation in the plane of the image in the case of the imaging of homocentric beams (symmetric 444 reflection of Mo $K\alpha$ radiation from a Si single crystal). The extinction length is $\Lambda = 34\ \mu$m, the radius of curvature is $R_x = 1$ m, the focal length is $F = 0.225$ m, and $L_h = 0.3$ m, and $y_{\rm eff} = 1$ mm.

holds between the radii of curvature, Eqs. (36) and (37) are the same, so the focal lines degenerate to a point (point-to-point focusing). Relation (38) and the condition that the diffraction geometry be symmetric constitute thus necessary and sufficient conditions; when these conditions are satisfied simultaneously, the imaging of x-ray beams occurs in a process in which homocentricity is preserved. The positions of the point source and of the image in the coordinates L_0, L_h are related by an equation which has the same form as the well-known thin-lens formula from ordinary optics:

$$1/L_0+1/L_h=1/F, \tag{39}$$

where the principal focal length F is

$$F={}^1/_2R_y/\sin\vartheta={}^1/_2R_x\sin\vartheta. \tag{40}$$

We now calculate the intensity distribution of the diffracted radiation near the imaging point. Substituting (16) into (19), and using (39), we find

$$I_h(\mathbf{r}_P)=|E_h(\mathbf{r}_P)|^2\sim4\left|J_1\left[\pi\Delta\xi_P^{-1}\left(\xi_P+\frac{L_h}{L_0}\xi_S\right)\right]\Big/\pi\Delta\xi_P^{-1}\left(\xi_P+\frac{L_h}{L_0}\xi_S\right)\right|^2\times\theta\left(\frac{\xi_P}{\alpha_hL_h}+\frac{\xi_S}{\alpha_hL_0}\right)\left|\sin\left[\pi\Delta y_P^{-1}\left(y_P+\frac{L_h}{L_0}y_S\right)\right]\Big/\pi\Delta y_P^{-1}\left(y_P+\frac{L_h}{L_0}y_S\right)\right|^2, \tag{41}$$

where the diffraction dimensions of the image in the plane perpendicular to the direction in which the diffracted wave is propagating are

$$\Delta\xi_P=\left|1-\frac{L_h}{R_x\sin\vartheta}\right|\Lambda\cos\vartheta,\qquad\Delta y_P=\frac{\lambda L_h}{y_{eff}}, \tag{42}$$

$J_1(t)$ is the Bessel function of real argument of index one, and $\theta(t)$ is the unit step function.

In the case in which we are interested here, of the imaging of homocentric x-ray beams, the lateral and longitudinal (in differential form) image magnifications are, respectively,

$$K_\xi=K_y=-L_h/L_0, \tag{43}$$

$$dL_h/dL_0=-L_h^2/L_0^2. \tag{44}$$

Figure 5 illustrates the situation with the intensity distribution $I_h(x_p, y_p)$ of diffracted Mo $K\alpha$ radiation for the symmetric 444 reflection from a biaxially curved silicon crystal, used as a spherical lens, with a focal length $F = 0.225$ m, with $L_h = 0.3$ m, and with diffraction dimensions $\Delta x_p \approx 7\ \mu$m, $\Delta y_p \sim 10^{-2}\ \mu$m of the image. Figure 6 shows the lateral magnification K as a function of L_0, the distance from the source to the crystal, for various values of the radius of curvature R_x.

We have been discussing monochromatic homocentric x-ray beams. We will now show that a nonzero wavelength spread of the primary beam does not lead to a blurring of the image; i.e., the image in the diffracted rays is achromatic. At a fixed position of the point source S, a change in the radiation wavelength, $\lambda\to\lambda+\delta\lambda$, is equivalent to a rotation of direction OS in Fig. 1 through an angle $\delta\varphi = (\delta\lambda/\lambda)\tan\vartheta$ from the exact Bragg position. The associated effective displacements of the position of the point of the source and of the point of the image are $\delta\xi_s = -L_0\delta\varphi$, $\delta\xi_p = L_h\delta\varphi$. As a result, the shift of the maximum of intensity distribution (41) in the approximation linear in $|\delta\varphi|\ll1$ vanishes, since we have

$$\delta\xi_P/L_h+\delta\xi_S/L_0=0,\quad \delta y_P=0. \tag{45}$$

In other words, under conditions of symmetric Bragg diffraction a biaxially curved crystal with radii of curvature related by $R_y = R_x\sin^2\vartheta$ is an achromatic diffraction lens which performs a point-to-point focusing of x-ray beams.

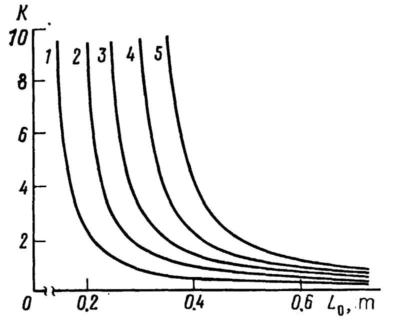

FIG. 6. Calculated values of the lateral magnification K of a spherical x-ray lens versus the distance L_0 for various radii of curvature R_x (in meters): 1—0.6; 2—0.8; 3—1.0; 4—1.2; 5—1.4 (symmetric 444 reflection of Mo $K\alpha$ radiation from single-crystal Si plate).

5. (PLANE WAVE)-TO-POINT FOCUSING

In the limiting case of the Bragg reflection of a plane-parallel beam, Eqs. (36) and (37) take the simple form

$$\gamma_h^2/L_h=(\gamma_0-\gamma_h)/R_x, \quad 1/L_h=(\gamma_0-\gamma_h)/R_y.$$

It follows immediately that a transition from an astigmatic diffracted beam to a homocentric beam is possible if the radii of curvature are related by

$$R_y=R_x\gamma_h^2. \tag{46}$$

In this case the focal plane lies at a distance

$$L_h^{(f)}=\gamma_h^2R_x/(\gamma_0-\gamma_h)=R_y/(\gamma_0-\gamma_h) \tag{47}$$

from the crystal. In the case of a symmetric Bragg-diffraction geometry, Eqs. (46) and (47) become the corresponding expressions derived in Ref. 8 for (plane wave)-to-point focusing.

Calculations similar to the derivation of (41) lead to the following expression for the intensity distribution of the diffracted radiation in the focal plane:

$$I_h(\mathbf{r}_P)\sim 4\left|J_1\left[\pi\Delta\xi_P^{-1}\left(\xi_P-\frac{\gamma_0|\gamma_h|R_x}{\gamma_0+|\gamma_h|}\delta\varphi_\xi\right)\right]\Big/\pi\Delta\xi_P^{-1}\left(\xi_P-\frac{\gamma_0|\gamma_h|R_x}{\gamma_0+|\gamma_h|}\delta\varphi_\xi\right)\right|^2$$
$$\times\theta\left(\xi_P-\frac{\gamma_0|\gamma_h|R_x}{\gamma_0+|\gamma_h|}\delta\varphi_\xi\right)\left|\sin\left[\pi\Delta y_P^{-1}\left(y_P+\frac{\gamma_0|\gamma_h|R_x}{\gamma_0+|\gamma_h|}\delta\varphi_y\right)\right]\Big/\pi\Delta y_P^{-1}\left(y_P+\frac{\gamma_0|\gamma_h|R_x}{\gamma_0+|\gamma_h|}\delta\varphi_y\right)\right|^2, \tag{48}$$

where the linear dimensions of the diffractive broadening of the focus, $\Delta\xi_p$, Δy_p, are

$$\Delta\xi_P=a\gamma_0|\gamma_h|\Lambda/(\gamma_0+|\gamma_h|), \quad \Delta y_P=\gamma_h^2\lambda R_x/(\gamma_0+|\gamma_h|)y_{eff}. \tag{49}$$

It can be seen from (48) that, depending on the angular deviations of the incident wave from the exact Bragg direction, the shift of the focusing point is given by

$$\delta\xi_P=\frac{\gamma_0|\gamma_h|R_x}{\gamma_0+|\gamma_h|}\delta\varphi_\xi, \quad \delta y_P=-\frac{\gamma_0|\gamma_h|R_x}{\gamma_0+|\gamma_h|}\delta\varphi_y. \tag{50}$$

Allowance for the wavelength spread of the radiation leads to the replacement of $\delta\varphi_\xi$ by $\delta\varphi_\xi+(1-|\gamma_h|/\gamma_0)\times(\delta\lambda/\lambda)\tan\vartheta$ in the first of expressions (50), as is easily shown.

It is appropriate to note here that this analysis of the $2D$ focusing of x rays has been carried out for the case of a slight curvature of the reflecting planes of the crystal. The reflection capability of such a crystal is described very accurately in terms of the small parameter, $|\nu|^{-1}\ll 1$ [see (15)], by the Fourier component of the Green's function of a perfect crystal, (16). On the other hand, all of the expressions which have been derived for the imaging of x-ray beams apply to a crystal of arbitrary curvature, used as a spherical lens, provided that the propagation of the diffracted radiation is described by eikonal function (20).

A (plane wave)-to-point focusing has recently been observed by Kushnir and Suvorov[9] in the case of diffractive backscattering of x-ray beams: $\vartheta\approx\pi/2$. Under the experimental conditions of Ref. 9, the focus lay at a distance $F=R_x/2=22.5$ cm from the crystal (Co $K\alpha$ radiation, $\lambda=1.79$ Å, 620 reflection from Ge); the diffractive broadening was $\Delta\xi_p\sim\frac{1}{4}\lambda\,|\chi_{620}^{(\mathrm{Ge})}|^{-1/2}\approx 120$Å; and the width of the Co $K\alpha$ line was $\delta\lambda/\lambda=3.5\cdot 10^{-4}$.

According to the DuMond diagram method,[1] the angular divergence of the Co $K\alpha$ radiation incident on a spherically curved Ge crystal is determined by the dispersions of the Si(111) monochromator crystal and of the Ge (620) mirror, and is given by

$$\delta\varphi_\xi\sim\delta\varphi_y\sim(\delta\lambda/\lambda)^{(\mathrm{Ge})}\,\mathrm{tg}(\vartheta_{111}^{(\mathrm{Si})}),$$

where the spectral width of the mirror is $(\delta\lambda/\lambda)^{(\mathrm{Ge})}=|\chi_{620}^{(\mathrm{Ge})}|=1.4\cdot 10^{-5}$. Substituting these values into (50), we find

$$\lambda\xi_P\sim\delta y_P\sim F(\delta\lambda/\lambda)^{(\mathrm{Ge})}\,\mathrm{tg}\,\vartheta_{111}^{(\mathrm{Si})}\approx 1\ \mu\mathrm{m}.$$

This result is about an order of magnitude smaller than the focus width found in Ref. 9, $\approx 10\ \mu$m, which was set by experimental errors, primarily irregularities at the surface of the Si(111) monochromator crystal and the Ge(620) spherical mirror.

The theoretical description of the focusing of x-ray beams by biaxially curved crystals proposed here can be used directly to solve other problems of interest in the field of x-ray optics, e.g., to analyze the properties of diffracted beams in the case of Bragg reflection from spatially modulated crystals: crystalline Fresnel zone plates,[16] crystals whose surface is deformed by a standing ultrasonic wave,[17] etc.

[1] R. Caciuffo, S. Melone, F. Rustichelli, and A. Voeuf, Phys. Rep. **152**, 3 (1987).
[2] G. Schmahl and D. Rudolph (editors), *X-Ray Microscopy*, Springer-Verlag, New York, 1984.
[3] F. N. Chukhovskiĭ, Metallofizika **2**, 3 (1980).
[4] F. N. Chukhovskiĭ, Metallofizika **3**, 3 (1981).
[5] D. W. Berreman, J. Stamatoff, and S. Kennedy, J. Appl. Opt. **16**, 2081 (1977).
[6] V. I. Kushnir, V. M. Kaganer, and E. V. Suvorov, Acta Cryst. A **41**, 17 (1985).
[7] L. V. Levonyan and M. K. Balyan, in: Second Conference on the All-Union Intercollegiate Complex Program Rentgen, Chernovtsy 1987, p. 99.
[8] K. T. Gabrielyan, D. I. Piskunov, F. N. Chukhovskiĭ, and G. O. Demirchyan, Pis'ma Zh. Eksp. Teor. Fiz. **46**, 411 (1987) [JETP Lett. **46**, 517 (1987)].
[9] V. I. Kushnir and É. V. Suvorov, Pis'ma Zh. Eksp. Teor. Fiz. **48**, 109 (1988) [JETP Lett. **48**, 117 (1988)].
[10] F. N. Chukhovskiĭ, K. T. Gabrielyan, and P. V. Petrashen', Dokl. Akad. Nauk SSSR **238**, 81 (1978) [Sov. Phys. Dokl. **23**, 52 (1978)].
[11] K. T. Gabrielyan, F. N. Chukhovskiĭ, and Z. G. Pinsker, Zh. Tekh. Fiz. **50**, 3 (1980) [Sov. Phys. Tech. Phys. **25**, 1 (1980)].
[12] V. L. Indenbom and F. N. Chukhovskiĭ, Usp. Fiz. Nauk **107**, 229 (1972) [Sov. Phys. Usp. **15**, 298 (1973)].
[13] V. M. Samsonov, Preprint No. 278, Leningrad Institute of Nuclear Physics, Leningrad, 1976.
[14] H. Johann, Z. Phys. **60**, 185 (1931).
[15] L. Hamos, Naturwissen. **20**, 705 (1932); Ann. Phys. (Leipzig) **17**, 716 (1933).
[16] V. V. Aristov, Yu. A. Basov, G. N. Kulipanov, *et al.*, Pis'ma Zh. Tekh. Fiz. **14**, 3 (1988) [Sov. Tech. Phys. Lett. **14**, 1 (1988)].
[17] S. Kikuta, T. Takahashi, and S. Nakatani, Jpn. J. Appl. Phys. **23**, L193 (1984).

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