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X-ray Diffraction Lenses with Spherical Focusing

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Abstract

X-ray spherical-wave focusing in multibeam dynamical diffraction by a biaxially bent single crystal has been considered. In contrast to cylindrical lenses already studied in the two-beam case, which presented a line focus, here wave packets focusing in two directions into a single point are dealt with. The conditions for focusing of the trajectories of the X-ray Bloch waves are established and the algorithm for the determination of the parameters of corresponding X-ray optical systems is described. Possible sets of parameters are calculated. The X-ray wave field distribution in a crystal is simulated numerically. The calculated topographs confirm the existence of the focusing effect.

1. Introduction

Optics for focusing X-rays and neutrons have been developed in two main directions – Fresnel zone plates for soft radiation (~40 Å) (Kirz, 1974; Kearney, Klein, Opat & Gähler, 1980) and diffraction lenses based on single crystals for hard radiation (~1 Å). The operation of such lenses is based on the effect of dynamical focusing of X-rays (or neutrons), which consists of the compression of coherent wave packets during dynamical scattering by single crystals. Until recently both theorists and experimenters have studied this effect mainly for two-beam diffraction (see references in the paper by Kushnir & Suvorov, 1982). In this case wave packets can be compressed by a crystal only in one direction determined by the

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diffraction vector, and therefore the corresponding lens is cylindrical and has a line focus.

Yet for the majority of practical applications, spherical focusing is required where wave packets are compressed by a crystal into a point and not into a line. Obviously, for the design of the corresponding X-ray optical system one should solve the three-dimensional problem of dynamical focusing, *i.e.* use multibeam noncoplanar diffraction. Baskakov & Zel'dovich (1978) have extended the idea of the diffraction focusing of X-ray Bloch waves in a double-crystal interferometer (Indenbom, Slobodetskii & Truni, 1974) to the multibeam case. It has been shown that the realization of such focusing for n-beam diffraction ($n \geq 3$) is possible while using a $2n$-crystal scheme (which meets serious experimental difficulties) with magnification equal to unity and resolution $\sim 10\ \mu m$, as in the two-beam case.

The problem of spherical-wave focusing by a perfect crystal has been studied theoretically (Homma, Ando & Kato, 1966; Kato, 1968; Afans'ev & Kohn, 1977) and experimentally (Aristov, Polovinkina, Shmyt'ko & Shulakov, 1978) for two beams and then extended to the multibeam case by Kohn (1977). In terms of geometrical optics (Kato, 1963, 1964) focusing of a spherical wave by a crystal can be realized because a curved sheet of the dynamical dispersion surface transforms a family of diverging trajectories of X-rays in vacuum into a family of converging trajectories of Bloch waves in the crystal. The multibeam dispersion surface is curved in two dimensions and therefore focuses beams in two directions but, generally speaking, at different depths (astigmatism). The conditions for focusing without astigmatism derived by Kohn (1977) consist of the compensation of the curvature tensors for dispersion surfaces of X-ray waves in vacuum and in the crystal. Yet Kohn gave no indication as to how these conditions could be realized. Magnification of such a lens is equal to unity, its resolution being $\sim 10\ \mu m$.

The aim of the present work is to extend the ideas of two-beam focusing by a bent crystal (Petrashen' & Chukhovskii, 1976; Kushnir & Suvorov, 1980) to the multibeam case. In the two-beam case, a crystal can be bent in such a way that the trajectories of the Bloch waves are still straight. This is achieved when the 'force' F (Kato, 1963, 1964) is equal to zero:

$$F = \frac{\partial^2(\mathbf{H}, \mathbf{u})}{\partial s_0 \partial s_1} = 0; \qquad (1)$$

then the waves propagate as in a nonbent crystal. The bend manifests itself in the fact that the curvature of the crystal surface partially compensates for the curvature of the spherical wave front, thus increasing the effective source–crystal distance. For usual source–crystal distances L(of the order of a meter), the effective distance L_{eff} can reach several hundred meters. Owing to the bend in the crystal, the magnification $K \simeq L_{\text{eff}}/L$ of such a lens differs from unity and reaches values up to 10^3, its resolution, $\Lambda \tan \theta / K$ (Λ is the extinction length and θ is the Bragg angle), being as high as 100 Å.

The present work considers possible ways of designing analogous lenses for multibeam focusing; such lenses are 'spherical' and not cylindrical and they focus waves in two directions. The crystal must be biaxially bent in such a way that the curvature of its surface should compensate for the curvature of the spherical wave front simultaneously in two directions; this condition immediately imposes limitations on the crystal orientation.

In § 2 the bending conditions which generalize (1) are described. The relation between the influence function of a crystal bent in the indicated way and the influence function for a plane crystal is then determined. In § 3 the problem of spherical-wave diffraction by a bent crystal is reduced to that of diffraction by a plane crystal; wave trajectories are determined and the caustic equation and conditions for focusing without astigmatism are derived. The requirements that should be met by the X-ray optical system of a diffraction lens are formulated. It is shown that the problem can be significantly simplified if the X-ray optical system has a symmetry plane. § 4 demonstrates how the requirements stated above can be met. The characteristics of the desired X-ray optical system are obtained and compared with the results of numerical simulation.

2. Multibeam dynamical diffraction by a bent crystal

If a diffraction lens is to form an image with high resolution, it should focus broad coherent wave packets. This requires that each beam at the exact Bragg position on the entrance surface of the crystal should form, due to diffraction, a coherent wave packet of maximum possible dimensions. But the deviation from the exact Bragg position varies over the crystal depth while the beam propagates in the bent crystal; a diffracted beam appears at a site where the deviation from exact Bragg angle is zero. Therefore, it is necessary that the Bragg condition should be satisfied for each beam over the whole crystal thickness.

Now, let us find the deviation from the Bragg position for a beam in a crystal having the displacement field $\mathbf{u}(\mathbf{r})$. The crystal polarizability χ is described by its Fourier series with terms

$$\chi_{\mathbf{H}} \exp[i\varphi(\mathbf{r})] \equiv \chi_{\mathbf{H}} \exp[i(\mathbf{H}^0, \mathbf{r} - \mathbf{u})], \qquad (2)$$

where $\mathbf{H}^0$ is the reciprocal-lattice vector for an ideal crystal. The effective local vector of the reciprocal lattice is changed according to the law

$$\mathbf{H} = \nabla\varphi = \mathbf{H}^0 - \nabla(\mathbf{H}^0, \mathbf{u}) \qquad (3)$$

and, consequently, the local deviation from the Bragg condition for a beam characterized by its wave vector $\mathbf{k}$ is also changed:

$$\delta[2(\mathbf{k}, \mathbf{H}) + \mathbf{H}^2] = -2(\mathbf{k} + \mathbf{H}^0, \nabla)(\mathbf{H}^0, \mathbf{u}). \quad (4)$$

The deviation is constant along the beam only if

$$(\mathbf{k}, \nabla)(\mathbf{k} + \mathbf{H}^0, \nabla)(\mathbf{H}^0, \mathbf{u}) = 0. \quad (5)$$

Equation (5) is the condition for the dynamical character of the scattering over the whole crystal to be maintained: for a beam incident at a given angle, the local deviation from the exact Bragg condition is constant and the beam experiences dynamical diffraction along its whole path through the crystal. In the two-beam case, (5) reduces to (1), which means that, in spite of the bending, the force affecting the ray trajectory in a crystal remains equal to zero. In the case of multibeam diffraction this condition should be satisfied for any pair of beams ($\mathbf{k}_j$ and $\mathbf{k}_l$ are the corresponding wave vectors satisfying exactly the Bragg law):

$$(\mathbf{k}_j, \nabla)(\mathbf{k}_l, \nabla)(\mathbf{k}_j - \mathbf{k}_l, \mathbf{u}) = 0. \quad (6)$$

Now let us determine the form of a wave field in a crystal, the deformation of which satisfies (6). For n-beam diffraction the X-ray field is a superposition of n strong waves:

$$\mathbf{D} = \sum_{j=1}^{n} \mathbf{D}_j^{(0)} \exp[i(\mathbf{k}_j, \mathbf{r})]. \quad (7)$$

The amplitudes $\mathbf{D}_j^{(0)}$ satisfy the Takagi (1969) equation:

$$2i(\mathbf{k}_j, \nabla)\mathbf{D}_j^{(0)} + k^2 \sum_{l=1}^{n} \chi_{jl}[\mathbf{D}_l^{(0)}]_j \exp[-i(\mathbf{H}_{jl}^0, \mathbf{u})] = 0, \quad (8)$$

where k is the magnitude of the wave vector in vacuum ($k = |\mathbf{k}_j|$): χ_{jl} are the Fourier components of the crystal polarizability; $\mathbf{H}_{jl}^0$ are the reciprocal-lattice vectors, $\mathbf{H}_{jl}^0 = \mathbf{k}_j - \mathbf{k}_l$; $[\mathbf{D}_l]_j$ is the projection of vector $\mathbf{D}_l$ onto the plane normal to $\mathbf{k}_j$.

Substituting

$$\mathbf{D}_j^{(0)} = \mathbf{D}_j^{(1)} \exp[-i(\mathbf{k}_j, \mathbf{u})] \quad (9)$$

into (8), we arrive at

$$2[i(\mathbf{k}_j, \nabla) + (\mathbf{k}_j, \nabla)(\mathbf{k}_j, \mathbf{u})]\mathbf{D}_j^{(1)} + k^2 \sum_{l=1}^{n} \chi_{jl}[\mathbf{D}_l^{(1)}]_j = 0.$$

The solution of the system is sought in the form

$$\mathbf{D}_j^{(1)} = \mathbf{D}_j^{(2)} \exp[i\Phi(\mathbf{r})], \quad (10)$$

where $\mathbf{D}_j^{(2)}(\mathbf{r})$ is the solution of the Tagaki equations for a plane crystal; $\Phi(\mathbf{r})$ is a real phase, independent of the label j of the beam. The value of the phase should be obtained through the set of equations

$$(\mathbf{k}_j, \nabla)\Phi = (\mathbf{k}_j, \nabla)(\mathbf{k}_j, \mathbf{u}) \equiv F_j. \quad (11)$$

The equality of the mixed derivatives

$$(\mathbf{k}_l, \nabla)F_j = (\mathbf{k}_j, \nabla)F_l \quad (12)$$

is a necessary condition for the existence of solutions to (11). This coincides with the conditions for the dynamical character of scattering (6).

If $n = 3$ (space dimensionality), (12) is also sufficient. For $n = 3$, the left side of (11) contains the derivatives along all three independent space directions $(\mathbf{k}_j, \nabla) = k\partial/\partial s_j$; (12) can be rewritten in the form $\mathrm{rot}_s\, \mathbf{F}_s = 0$, where subscript s denotes the vector operations in space (s_1, s_2, s_3) and vector $\mathbf{F}_s$ denotes the set of components F_j. Since a vector whose curl is zero can be represented in the form of the gradient of a certain scalar Φ, $\mathbf{F}_s = \mathrm{grad}_s\, \Phi$. This equality coincides with (11) and proves the existence of the solution for the system.

If $n \geq 4$, the number of equations in (11) exceeds the number of unknowns. Operators $(\mathbf{k}_j, \nabla)$ for $n \geq 4$ can be represented by linear combinations of $\partial/\partial s_i$ ($i = 1, 2, 3$); then for the consistency of (11) it is necessary that the right-hand sides of the corresponding equations can be represented by the same linear combinations of the right-hand sides of the first three equations. These conditions can be met, for example, if the problem possesses a certain symmetry.

Now, let us determine the explicit form of phase Φ for a uniformly bent thin parallel plate. In this case the displacement $\mathbf{u}(\mathbf{r})$ is a quadratic function of coordinates and therefore the components $\varepsilon_{\alpha\beta}$ of the strain tensor are, in the isotropic approximation, proportional to z (Landau & Lifshits, 1969, § 11) (z being the coordinate normal to the surface of the plate); the corresponding proportionality coefficients $\varepsilon_{\alpha\beta}(z)/z$ are constant along the whole plate, *i.e.* independent of coordinates x and y. The components of the stress tensor $\sigma_{\alpha\beta}$ are also proportional to z and, according to Sirotin & Shaskol'skaya (1979, § 53), will also be proportional to z for the case of an arbitrary anisotropy. Thus, the quantities $F_j = k_{j\alpha}k_{j\beta}\varepsilon_{\alpha\beta}$ are also proportional to z: $F_j = f_j z$, where f_j are coordinate independent. The solution of (11) has the form $\Phi = C_0 z^2/2$, where

$$C_0 = \frac{f_1}{k_{1z}} = \frac{f_2}{k_{2z}} = \ldots = \frac{f_n}{k_{nz}}. \quad (13)$$

The uniform bend of a thin plate is fully determined by three parameters, namely the main radii of the surface curvature for the plate and the orientation of the main normal sections (see Appendix). If $n = 3$, two independent conditions of the type (13) fully determine the orientation of the main normal sections and the ratio of the main curvature radii. If $n \geq 4$, the uniform bend satisfying the conditions of dynamical scattering (6) is possible only if among $(n-1)$ conditions (13) only two are independent. Thus, in the case of a uniformly bent crystal and under the conditions of dynamical scattering (6), the solutions of Takagi equations (8) have the form

$$\mathbf{D}_j^{(0)} = \mathbf{D}_j^{(2)} \exp\{i[C_0 z^2/2 - (\mathbf{k}_j, \mathbf{u})]\}, \qquad (14)$$

where $\mathbf{D}_j^{(2)}$ are the solutions for a plane crystal.

From this the relation between the influence function for the bent crystal, $\mathbf{G}_j^b(\mathbf{r}_0, \mathbf{r})$ (describing the amplitude of the jth beam at point $\mathbf{r}_0$ inside the crystal illuminated by a narrow beam at point $\mathbf{r}$ of the entrance surface), and the corresponding multibeam influence function for the plane crystal $\mathbf{G}_j^p(\mathbf{r}_0 - \mathbf{r})$ can be obtained:

$$\mathbf{G}_j^b(\mathbf{r}_0, \mathbf{r}) = \mathbf{G}_j^p(\mathbf{r}_0 - \mathbf{r}) \exp[i(C_0 z^2/2 - (\mathbf{k}_j, \mathbf{u}))|_{\mathbf{r}}^{\mathbf{r}_0}]. \qquad (15)$$

3. Spherical wave focusing

We now consider the multibeam diffraction of a spherical wave from a biaxially bent crystal and determine the conditions for the wave to be focused by the crystal. Let a spherical wave from a point source S fall on a biaxially bent parallel-sided single-crystal plate (Fig. 1) so that the Bragg conditions are fulfilled for n-wave noncoplanar diffraction. We assume the plate to be thin (*i.e.* thickness is much less than the two other dimensions) and uniformly bent (with a constant strain gradient). The shape of the surface for a biaxially bent plate is described by the expression

$$u_z|_{z=0} = -\left(\frac{x^2}{2R_x} + \frac{y^2}{2R_y} + \beta xy\right), \qquad (16)$$

where x and y are the coordinates along the surface

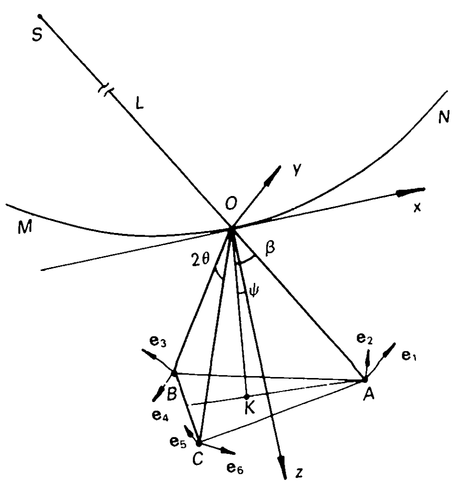


Fig. 1. X-ray optical system for a diffraction lens. S is the point source, MON is the bent entrance surface of a crystal, Oz is normal to this surface at a point O; $OABC$ is the Borrmann pyramid appearing during illumination of point O by a narrow beam; OK is the normal to the plane ABC forming equal angles β with OA, OB and OC; $\mathbf{e}_1 - \mathbf{e}_6$ are the unit vectors of the polarization, θ is the Bragg angle, ψ is the angle between OK and Oz.

of the nonbent plate, while three parameters $1/R_x$, $1/R_y$ and β characterize the bending. The phase of a spherical wave varies along the bent surface of the crystal $\mathbf{r}' = \mathbf{r} + \mathbf{u}(\mathbf{r})$; $\mathbf{r} = (x, y, 0)$ according to the law

$$\varphi_s(\mathbf{r}) = k|\mathbf{r}' - \mathbf{r}_s| = (\mathbf{k}_1, \mathbf{r}) + (Ax^2 + 2Bxy + Cy^2)/2, \qquad (17)$$

where

$$A = k\left(\frac{1-\gamma_x^2}{L} - \frac{\gamma_z}{R_x}\right), \qquad B = k\left(\frac{\gamma_x\gamma_y}{L} - \gamma_z\beta\right),$$

$$C = k\left(\frac{1-\gamma_y^2}{L} - \frac{\gamma_z}{R_y}\right),$$

$\mathbf{r}_s$ is the radius vector of the source S, L is the distance between the source S and point O, γ_x, γ_y, γ_z are the direction cosines of the wave vector $\mathbf{k}_1$ of the incident beam.

The wave field inside the crystal is described by the convolution of the incident spherical wave with the influence function

$$\mathbf{D}(\mathbf{r}_0) \propto \sum_{j=1}^{n} \iint \exp[i\varphi_s(\mathbf{r})]\mathbf{G}_j^b(\mathbf{r}_0, \mathbf{r}) \times \exp[i(\mathbf{k}_j, \mathbf{r}_0 - \mathbf{r}')]\,\mathrm{d}x\,\mathrm{d}y. \qquad (18)$$

Substituting $\mathbf{r}' = \mathbf{r} + \mathbf{u}(\mathbf{r})$, using (15) (in order to introduce the influence function for a plane crystal), and omitting the constant phase factors, we arrive at

$$\mathbf{D}(\mathbf{r}_0) \propto \sum_{j=1}^{n} \iint \exp[i(Ax^2 + 2Bxy + Cy^2)/2] \times \mathbf{G}_j^p(\mathbf{r}_0 - \mathbf{r})\,\mathrm{d}x\,\mathrm{d}y. \qquad (19)$$

Thus, the problem of the diffraction of a spherical wave by a bent crystal reduces to that of diffraction by a plane crystal but with different boundary conditions (17) and additional degrees of freedom, namely the bending parameters of the entrance surface of the crystal. Since the explicit form of the multibeam influence function for a perfect crystal is not known, it is more convenient to expand the incident wave in plane waves and determine the focusing conditions in terms of the dispersion surface of a perfect crystal.

In a perfect crystal a plane incident wave generates the set of Bloch waves. It is convenient to introduce, for each beam, two polarization vectors $\mathbf{e}$, normal to the corresponding wave vector $\mathbf{k}_j$ (our choice of the polarization unit vectors coincides with that of Baskakov & Zel'dovich (1978) and is shown in Fig. 1) and to arrange the components of vectors $\mathbf{D}_j$ (obtained from the expansion with respect to these polarizations) in a single-column vector of dimensionality $2n$. Then the eigenfunctions of the Takagi equations for a perfect crystal (Bloch waves) can be written in the form

$$\mathbf{V}(p, q) \exp[i(px + qy + s(p, q)z)],$$

where $\mathbf{V}$ is the vector column of dimensionality $2n$ and p and q are determined by the deviation of the incident plane wave from the exact Bragg conditions. Substituting this expression into the Takagi equations (8) and assuming a zero value of the displacement field ($\mathbf{u} \equiv 0$), we obtain the system of equations which determines $\mathbf{V}(p, q)$ and $s(p, q)$:

$$[\hat{H}(p, q) - s\hat{Q}]\mathbf{V} = 0; \tag{20}$$

the components of the matrices $\hat{H}$ and $\hat{Q}$ can be written as

$$H_{jl} = \frac{k^2}{2}\chi_{jl}(\mathbf{e}_j, \mathbf{e}_l) - \delta_{jl}(k_{jx}p + k_{jy}q);$$

$$Q_{jl} = k_{jz}\delta_{jl},$$

where $\mathbf{e}_j$ are the polarization unit vectors, subscripts j and l run over the values $1, 2, \ldots, 2n$, the component of each of the n wave vectors of the problem entering the diagonal elements twice in succession. Pre- and postmultiplication of the matrix involved in (20) by the diagonal matrix with components $T_{jl} = \delta_{jl}/k_{jz}^{1/2}$ leads to the equivalent system of equations

$$(\hat{U} - s\hat{E})\mathbf{W} = 0, \tag{21}$$

where $\hat{U} = \hat{T}\hat{H}\hat{T}$, $\mathbf{W} = \hat{T}^{-1}\mathbf{V}$, $\hat{E}$ being the unitary matrix. All the $2n$ eigenvalues $s_m(p, q)$ ($m = 1, 2, \ldots, 2n$) of the symmetrical matrix $\hat{U}$ are real and determine $2n$ sheets of the dispersion surface. The corresponding eigenvectors $\mathbf{W}_m(p, q)$ are orthogonal and can be chosen in such a way that

$$(\mathbf{W}_j, \mathbf{W}_l) = \delta_{jl}.$$

The vectors $\mathbf{V}_m$ are orthogonal with the 'weight' $\hat{Q}$:

$$(\mathbf{V}_j, \hat{Q}\mathbf{V}_l) = \delta_{jl}.$$

Now, using the Fourier transformation of convolution (19), we may proceed to the summation of Bloch waves

$$\begin{aligned}\mathbf{D}(x, y, z) = \sum_{m=1}^{2n} &\iint (\mathbf{V}_m, \hat{Q}\mathbf{D}_s)\mathbf{V}_m \\ &\times \exp\left[i(\tfrac{1}{2}ap^2 + bpq + \tfrac{1}{2}cq^2 + px + qy \right. \\ &\left. + s_m z)\right] \mathrm{d}p\, \mathrm{d}q, \end{aligned} \tag{22}$$

where $\mathbf{D}_s$ is the amplitude of the incident spherical wave (the incident beam is considered to be the first, so that the two first components of the column vector $\mathbf{D}_s$ have non-zero values). Parameters a, b and c of the Fourier transform of the incident spherical wave are related to parameters A, B and C in (17) by the expression

$$\begin{pmatrix} a & b \\ b & c \end{pmatrix} = -\begin{pmatrix} A & B \\ B & C \end{pmatrix}^{-1}. \tag{23}$$

The stationary-phase conditions for (22) lead for each sheet of the dispersion surface to the trajectory equations $x = x(z)$, $y = y(z)$ for the beam corresponding to the point (p, q) of the dispersion surface:

$$\begin{aligned} ap + bq + x + s_p z &= 0 \\ bp + cq + y + s_q z &= 0, \end{aligned} \tag{24}$$

where s_p and s_q are the corresponding partial derivatives, the subscript m of the chosen dispersion surface sheet being omitted. Now, let us find the caustics for the rays described by (24). For that, we calculate the trajectory displacement at a depth z caused by a small displacement $(\mathrm{d}p, \mathrm{d}q)$ of the excitation point (p, q) on the dispersion surface; the condition for zero displacement of the trajectory indicates that, at a given point, the trajectory is in contact with the caustic:

$$\begin{aligned}\begin{pmatrix} \mathrm{d}x \\ \mathrm{d}y \end{pmatrix} &= \hat{M}(z)\begin{pmatrix} \mathrm{d}p \\ \mathrm{d}q \end{pmatrix} \\ &\equiv -\left[z\begin{pmatrix} s_{pp} & s_{pq} \\ s_{pq} & s_{qq} \end{pmatrix} + \begin{pmatrix} a & b \\ b & c \end{pmatrix}\right]\begin{pmatrix} \mathrm{d}p \\ \mathrm{d}q \end{pmatrix} = 0. \end{aligned} \tag{25}$$

The condition for the existence of solutions, *i.e.* $\det \hat{M}(Z) = 0$, determines two values of $z^c_{1,2}(p, q)$ corresponding to focusing of the bundle of trajectories in two perpendicular directions, at different depths (astigmatism); the values of $z^c_{1,2}(p, q)$ together with (24) determine, in the parametric form, two sheets of the caustic corresponding to the given sheet of the dispersion surface. For each of the values of $z^c_{1,2}$, (25) determine the values of $\mathrm{d}p/\mathrm{d}q$; this in turn determines, in the plane (p, q), two local directions $\boldsymbol{\tau}_{1,2}(p, q)$ such that the displacement of the point (p, q) along the dispersion surface in these directions results in the intersection of the corresponding trajectories at a depth $z^c_{1,2}$. Focusing without astigmatism at depth t occurs when the focus depths are equal, $z^c_1 = z^c_2 = t$. This condition reduces to $\hat{M}(t) = 0$ either when the main radii of the curvature of the dispersion surface are of the same sign or when the problem has a symmetry plane. In both cases, the focusing without astigmatism conditions reduces to

$$\begin{pmatrix} A & B \\ B & C \end{pmatrix} = -\begin{pmatrix} a & b \\ b & c \end{pmatrix}^{-1} = \frac{1}{t}\begin{pmatrix} s_{pp} & s_{pq} \\ s_{pq} & s_{qq} \end{pmatrix}^{-1}. \tag{26}$$

On the other hand, the caustic may have a singularity if the derivative of $z^c_i(p, q)$ ($i = 1$ or 2) along the direction $\boldsymbol{\tau}_i(p, q)$ is equal to zero. Obviously, the brightest focus is formed if both conditions are fulfilled simultaneously: the condition for focusing without astigmatism (26) and the condition for the formation of a singularity on the caustic.

The problem of focusing is significantly simplified if the X-ray optical system has a plane of symmetry. Let the x axis lie along the symmetry plane and the y axis be normal to it. Then R_x and R_y are the main radii of the curvature of the crystal entrance surface (17) and $\beta = 0$. Among the conditions of dynamical scattering (6) only one remains independent, this condition determines the allowed value of the ratio R_x/R_y for a given orientation. The source (Fig. 1) is in the symmetry plane and therefore $\gamma_y = 0$. The dispersion surface also possesses a plane of symmetry, *i.e.* $s_m(p, q) = s_m(p, -q)$. The sought-for focus is such that $q = 0$ and $s_{pq}(p, 0) = 0$. The conditions of trajectory focusing (26) reduce to

$$k\left(\frac{1-\gamma_x^2}{L} - \frac{\gamma_z}{R_x}\right) = \frac{1}{ts_{pp}}, \qquad k\left(\frac{1}{L} - \frac{\gamma_z}{R_y}\right) = \frac{1}{ts_{qq}}, \quad (27)$$

where derivatives s_{pp} and s_{qq} are calculated at point $(p_F, 0)$ of the dispersion surface chosen for focusing. This point is determined by the condition for the formation of a singularity on the caustic

$$s_{ppp}(p_F, 0) = 0. \quad (28)$$

In the next section it will be shown how it is possible to satisfy simultaneously conditions (6), (27) and (28) in the case of three-beam diffraction.

4. Focusing in the three-beam case

Consider the problem of focusing in the three-beam case when the X-ray optical system has a plane of symmetry. The diffraction vectors must be chosen so as to form an isosceles triangle with a base of $\langle 110 \rangle$ type. Fig. 2 shows the dispersion surface for this case.

Now let us define the angle ψ, which is the angle between the normal to the ABC plane and the normal to the crystal surface (Fig. 1), the plane of symmetry being preserved. For this we should estimate the orders of magnitude of the terms in (27). Since $s_{pp} \sim s_{qq} \sim 1/(k\chi)$, we obtain, for distances appropriate for the experimental realization of focusing ($L = 1$ m, $t = 200\ \mu\text{m}$) the value $k/L \geq 100/(ts_{pp})$. Thus, the two terms on the left-hand sides of (27) should almost compensate for each other; in other words, the crystal bend should almost compensate for the curvature of the incident wave front. The condition of complete

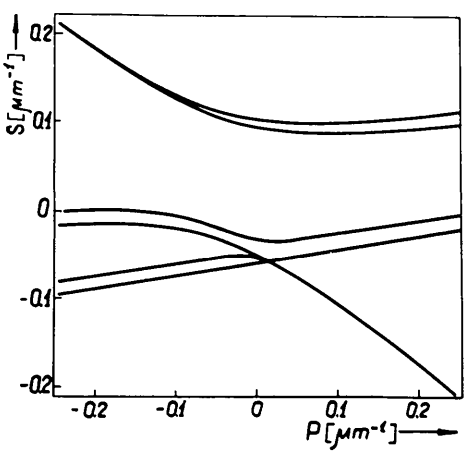


Fig. 2. The sections of the dispersion surface at the plane of symmetry in the three-beam case. 331, 313 reflections, Mo $K\alpha$ radiation.

compensation of the curvatures $R_y/R_x = 1 - \gamma_x^2$ together with (6) determine a certain angle ψ_0; the tilt angle chosen for the realization of focusing should only differ slightly from ψ_0. Note that the parameters of the calculated X-ray optical systems strongly depend on the difference $\psi - \psi_0$.

Setting the tilt angle ψ and using the expressions derived in the Appendix, one can calculate the elastic field $\mathbf{u}(\mathbf{r})$ depending on R_x and R_y; then the condition of dynamical scattering (6) will determined the ratio R_x/R_y. At a given ψ the condition for the appearance of a singularity on the caustic (28) determines the desirable point p_F of the dispersion surface and the values of $s_{pp}(p_F, 0)$ and $s_{qq}(p_F, 0)$. To determine these derivatives numerically it is convenient, as was suggested by Kohn (1976), to invoke the perturbation theory. Then

$$s_p^{(m)}(p, q) = \langle \mathbf{W}_m | \partial \hat{U}/\partial p | \mathbf{W}_m \rangle,$$

$$s_{pp}^{(m)}(p, q) = 2 \sum_{j \neq m} \frac{(\langle W_m | \partial \hat{U}/\partial p | \mathbf{W}_j \rangle)^2}{s_m - s_j}.$$

Similar expressions can also be written for other derivatives. Here, $s_m(p, q)$, and $\mathbf{W}_m$ are the eigenvalues and eigenvectors of (21), respectively, calculated at point (p, q). In the derivation we have used the fact that matrix $\hat{U}$ linearly depends on p and q:

$$\partial U_{jl}/\partial p = -\delta_{jl} k_{jx}/k_{jz}.$$

Since multiplication of quantities R_x, R_y, L and t by the same factor does not change the focusing conditions, one of these quantities, say t, can be set arbitrarily. Then the focusing conditions (27) for trajectories determine the quantities L, R_x and R_y, thus leading to the determination of still unknown parameters of the sought-for X-ray optical system.

Now the only problem left is the determination of the lens magnification. When the source is displaced, the direction SO (Fig. 1) of the wave vector $\mathbf{k}$ of the incident wave is different from that of the wave vector $\mathbf{k}_1$, which satisfies the exact Bragg condition. This results in the appearance of an additional term $(\mathbf{k} - \mathbf{k}_1, \mathbf{r})$ in expansion (17) of the spherical wave phase. Relating the difference $\mathbf{k} - \mathbf{k}_1$ to the source displacement in directions x and y one can readily obtain the corresponding displacement of the focus and, thus, calculate the magnification coefficients in directions x and y:

$$K_x = \left(1 - \frac{L}{\gamma_z R_x}\right)^{-1}, \qquad K_y = \left(1 - \frac{\gamma_z L}{R_y}\right)^{-1}. \quad (29)$$

For a nonbent crystal the problem is translation invariant in the (x, y) plane and the magnification coefficients are equal to unity. Bending the crystal, we can reach the value $K \gtrsim 100$ (see below).

As an example let us calculate the parameters for an X-ray optical system for 331, 313 Mo $K\alpha$ diffraction from a silicon crystal. Here $\psi_0 = -11{\cdot}481$ mrad;

Table 1. *Distributions of wavefields in a crystal*

Thickness $t = 200$ μm in all cases;

Radiation	Reflections	Branch number	Polarization*	L (mm)	R_x (mm)	R_y (mm)	ψ (rad)	Magnification K_x	Magnification K_y	z_F (μm)
Mo $K\alpha$	$331, 3\bar{1}\bar{3}$	1	1, 4	201	220	190	−0·01066	62·6	81·4	174
		2	2, 3	201	219	189	−0·01042	61·3	86·5	170
		2	2, 3	401	445	382	−0·009335	30·7	43·3	
	$224, \bar{2}\bar{2}4$	1	1, 4	197	220	181	0·02700	73·5	114	205
	$311, \bar{1}\bar{3}1$	1	2, 3	206	249	174	0·1490	91·8	139	216
Ag $K\alpha$	$331, 3\bar{1}\bar{3}$	1	1, 4	201	212	190	−0·02564	62·5	76·6	158
	$224, \bar{2}\bar{2}4$	1	1, 4	211	226	202	0·01197	68·6	87·2	179
	$224, 2\bar{4}\bar{2}$	1	2, 3	200	234	173	0·006152	225	369	200

* Polarizations in incident and diffracted beams.

if ψ is chosen in such a way that $L/t \simeq 1000$ ($\psi = -10{\cdot}42$ mrad) and $t = 200$ μm, the source-crystal distance calculated by the above algorithm is $L = 20{\cdot}1$ cm, and the curvature radii are $R_x = 21{\cdot}9$ and $R_y = 18{\cdot}9$ cm. Fig. 3 shows the caustic sheets corresponding to such an X-ray optical system. The sheets touch each other at a point where one of them has a singularity. The magnification coefficients are $K_x = 61{\cdot}3$ and $K_y = 86{\cdot}5$.

For the calculated X-ray optical system we have obtained the distributions of wave fields in a crystal. The fields were calculated as the superposition of the solutions of the plane-wave problem (21) in the form of integral (22) over the dispersion surface, the summation being carried out over all its sheets. The calculations proved that the focus (a point with the maximum intensity) does not coincide with the singularity on the caustic surface but lies at a slightly different depth z_F (Table 1). These discrepancies are due to two different factors: firstly, the shape of the chosen sheet of the dispersion surface differs from a parabaloid and, secondly, the contributions to the intensity also come from other Bloch waves (other branches of the dispersion surface). The intensity distribution in the region of focusing is shown in Fig. 4. Figs. 5(a),(b) and (c) show the intensity distributions for sections parallel to the xz, yz and xy planes passing through the focus. The first two sections of the crystal are normal to its entrance and exit surfaces, the third one coinciding with the exit surface (a topograph). The incident wave was taken to be polarized in the $\mathbf{e}_2$ direction, and the intensity of the diffracted wave polarized in the $\mathbf{e}_3$ direction was calculated.

The results of the calculations (Figs. 4 and 5) show that, for this X-ray optical system and with the parameters found, the incident spherical wave experiences a diffraction compression (focusing); the focus width at midheight is $\Delta f_x = 15$ and $\Delta f_y = 9$ μm and the shape of the focus is close to elliptic with the semiaxis ratio of 1·67. At magnifications $K_x = 61{\cdot}3$ and $K_y = 86{\cdot}5$ the resolution in the object plane is

$$\Delta\xi_x = \Delta f_x / K_x = 0{\cdot}24, \qquad \Delta\xi_y = \Delta f_y / K_y = 0{\cdot}10 \ \mu\text{m}.$$

The values are approximately equal to the diffraction resolution limit of a circular lens with diameter $d_B =$

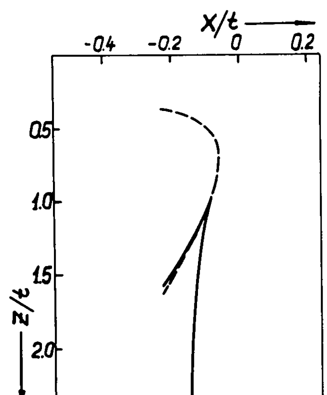


Fig. 3. Section at the xz plane of symmetry of the caustic surface corresponding to the second (from top) sheet of the dispersion surface shown in Fig. 2. The solid line corresponds to beam focusing in the plane of the drawing, dashed line to that in the normal direction.

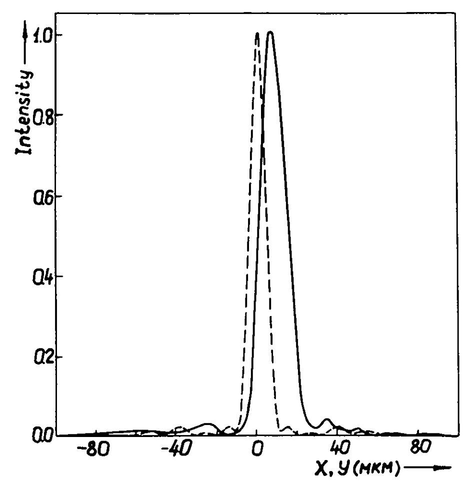
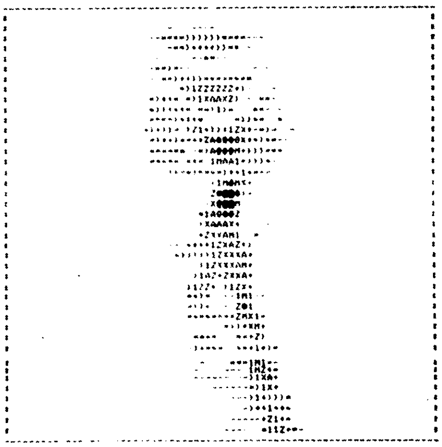


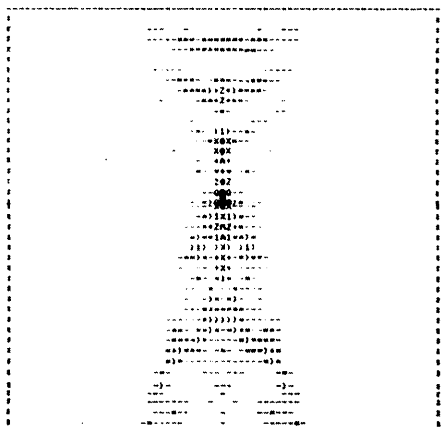
Fig. 4. Intensity distributions of a diffracted beam along the lines parallel to x (solid line) and y (dashed line) axes passing through the focus (for parameters see Table 1, line 4).

73 μm, inscribed into the base of the Borrmann pyramid:

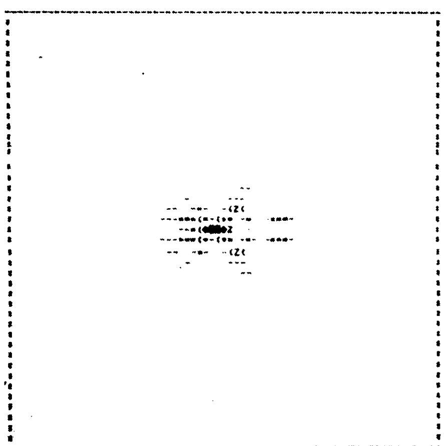
$$\Delta\xi = \lambda\Lambda/d_B \simeq 0{\cdot}19\ \mu\text{m}.$$



(a)



(b)



(c)

Fig. 5. Intensity distribution of a diffracted beam in sections parallel to planes (a) xz, (b) yz, and (c) xy passing through the focus (for parameters see Table 1, line 2).

Of course, the inverse X-ray optical system (with the source at the crystal surface and the focus far from it, near the center of curvature) should operate as a reducing lens ($K_x = 1/61{\cdot}3$ and $K_y = 1/86{\cdot}5$) with the focus dimensions $\Delta f_x = 0{\cdot}24$ and $\Delta f_y = 0{\cdot}10$ μm.

The results obtained show that a biaxially bent single crystal can operate as a spherically focusing X-ray lens having a magnification different from unity, if the following requirements are met.

1. Scattering in a bent crystal is maintained to be dynamical.
2. The trajectories are focused into a point without astigmatism.
3. The caustic surface has a singularity at the same point.

The presence of a plane of symmetry in the X-ray optical system simplifies the problem and permits one to calculate all the parameters of the system (Table 1).

Though aberrations displace a point with the maximum intensity in the crystal relative to the caustic singularity, the dimensions of the focus obtained are close to the diffraction limit. Thus, dynamical focusing in multibeam diffraction from bent crystals could be used in the designing of new focusing elements for coherent X-ray and neutron optics.

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APPENDIX

Displacement field in a uniformly bent crystal

As has already been noted, we restrict ourselves to the consideration of a uniformly bent crystal where all the components of stress and strain tensors are proportional to coordinate z:

$$\sigma_{ij} = \sigma^0_{ij} z/t, \qquad \varepsilon_{ij} = \varepsilon^0_{ij} z/t. \qquad (30a,b)$$

The coefficients of proportionality are coordinate independent. The most general form of the displacement field satisfying (30b) is

$$\begin{aligned} u_x &= \frac{xz}{R_x} + \beta yz + \alpha_x \frac{z^2}{2} \\ u_y &= \frac{yz}{R_y} + \beta xz + \alpha_y \frac{z^2}{2} \qquad (31) \\ u_z &= -\left(\frac{x^2}{2R_x} + \frac{y^2}{2R_y} + \beta xy + \alpha_z \frac{z^2}{2}\right). \end{aligned}$$

Parameters α_x and α_y are the curvatures of the atomic planes with normals x and y, respectively; α_z is related to nonuniform extension and compression of a material of the plate along the z axis; parameters R_x, R_y, and β describe the shape of the bent plate surface (16) and therefore their assignment fully determines the displacement field. We shall now determine the relation between these parameters and the three other parameters α_x, α_y and α_z. We express them *via* constants ε^0_{ij}:

$$\begin{aligned} t/R_x &= \varepsilon^0_{xx} & t\alpha_x/2 &= \varepsilon^0_{xz} \\ t\beta &= \varepsilon^0_{xy} & t\alpha_y/2 &= \varepsilon^0_{yz} \\ t/R_y &= \varepsilon^0_{yy} & -t\alpha_z &= \varepsilon^0_{zz}. \end{aligned} \tag{32}$$

The boundary conditions on the plate surface with normal z have the form (Landau & Lifshits, 1965)

$$\sigma_{xz} = \sigma_{yz} = \sigma_{zz} = 0.$$

Therefore, the components of a strain tensor may be expressed *via* the three remaining components of the stress tensor:

$$\begin{pmatrix} \varepsilon_{xx} \\ \varepsilon_{xy} \\ \varepsilon_{yy} \end{pmatrix} = \hat{S}_1 \begin{pmatrix} \sigma_{xx} \\ \sigma_{xy} \\ \sigma_{yy} \end{pmatrix}, \qquad \begin{pmatrix} \varepsilon_{xz} \\ \varepsilon_{yz} \\ \varepsilon_{zz} \end{pmatrix} = \hat{S}_2 \begin{pmatrix} \sigma_{xx} \\ \sigma_{xy} \\ \sigma_{yy} \end{pmatrix}. \tag{33}$$

Here the known and unknown components of the strain tensor are arranged for convenience in two separate column vectors. Matrices $\hat{S}_1$ and $\hat{S}_2$ are related to tensor $\hat{S}$ of elastic compliance constants:

$$\begin{aligned} \hat{S}_1 &= \begin{pmatrix} S_{xxxx} & 2S_{xxxy} & S_{xxyy} \\ S_{xyxx} & 2S_{xyxy} & S_{xyyy} \\ S_{yyxx} & 2S_{yyxy} & S_{yyyy} \end{pmatrix}, \\ \hat{S}_2 &= \begin{pmatrix} S_{xzxx} & 2S_{xzxy} & S_{xzyy} \\ S_{yzxx} & 2S_{yzxy} & S_{yzyy} \\ S_{zzxx} & 2S_{zzxy} & S_{zzyy} \end{pmatrix}. \end{aligned} \tag{34}$$

The factor 2 here takes into account the contribution of stresses σ_{xy} and σ_{yx} to the deformation.

In turn, the components of tensor $\hat{S}$ in the chosen reference system depend on the plate orientation and can be expressed *via* tensor $\hat{S}^0$ in the crystal-physical reference system (see, for example, Sirotin & Shaskol'skaya, 1979):

$$S_{ijkl} = S^0_{\alpha\beta\gamma\delta} g_{i\alpha} g_{j\beta} g_{k\gamma} g_{l\delta}, \tag{35}$$

where $\hat{g}$ is the ψ-dependent matrix of transition between the two reference systems; all the indices run over the values x, y and z, the summation being taken over the repeating indices.

For cubic crystals, tensor $\hat{S}^0$ is fully determined by three elastic constants S_{11}, S_{12} and S_{44}:

$$S^0_{ijkl} = \begin{cases} S_{11} \text{ if } i=j=k=l \\ S_{12} \text{ if } i=j\neq k=l \\ S_{44}/4 \text{ if } i=k\neq j=l \text{ or } i=l\neq j=k \\ 0 \text{ in all the remaining cases.} \end{cases} \tag{36}$$

Relations (34)–(36) fully determine the matrices $\hat{S}_1$ and $\hat{S}_2$, and from (32) and (33) the sought-for relation between the parameters of the displacement field can readily be obtained:

$$\begin{pmatrix} \alpha_x/2 \\ \alpha_y/2 \\ -\alpha_z \end{pmatrix} = \hat{S}_2 \hat{S}_1^{-1} \begin{pmatrix} 1/R_x \\ \beta \\ 1/R_y \end{pmatrix}. \tag{37}$$

In § 3 we have described an X-ray optical system having the symmetry plane xz. In this case $\alpha_y = \beta = 0$ and the matrices $\hat{S}_1$ and $\hat{S}_2$ can be reduced to the form 2×2.

All the parameters of the displacement field being determined the coefficients f_j in the conditions of dynamical scattering (13) can be determined as

$$f = \frac{k_x^2}{R_x} + \frac{k_y^2}{R_y} + 2\beta k_x k_y + k_z(\alpha_x k_x + \alpha_y k_y - \alpha_z k_z). \tag{38}$$

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