Lateral displacement of Bragg-reflected x-ray beams

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In the usual treatment of the dynamical diffraction of x rays, one considers a plane wave which is incident on a crystal giving rise to a reflected plane wave. This work extends that theory by considering an incident bounded beam of x rays. We evaluate the resulting Bragg-reflected beam for both symmetric and asymmetric reflections and show that the reflected beam undergoes a lateral shift and that incidence at the edges of the range of total reflection results in a lateral wave traveling along the surface. This is analagous to the Goos-Hanchen effect for total internal reflection of an optical beam. In addition, if the incident beam is spectrally wide, the reflected beam is distorted and broadened, as well as shifted.

I. INTRODUCTION

It is well known in optics that when a bounded beam undergoes total internal reflection, the reflected beam is laterally displaced from the position predicted by geometric optics and may exhibit an altered cross-sectional energy distribution as described in Refs. 1–6. This so-called Goos-Hanchen effect arises because a bounded beam consists of waves which are incident at slightly different angles and which are reflected with different phases. The superposition of these reflected waves results in a reflected beam which is the sum of the wave expected from geometric optics and a lateral wave which travels along the surface and radiates energy in the reflected direction (the faint "trailing illumination"). The phase difference between the geometric and lateral waves is such that they destructively interfere to the left of the axis of geometric reflection and constructively interfere to the right, resulting in a shift of the axis to the right. This is illustrated in Fig. 1 where d is the beam shift along the surface and d^r is the shift perpendicular to the beam axis.

One would expect that a bounded x-ray beam which undergoes dynamical Bragg reflection will exhibit similar effects since the phase of dynamically reflected waves differ for slightly different angles of incidence. Because the location and shape of the reflected x-ray beam may be used to yield information about the crystal, it is important to understand what distortions may be introduced by the boundedness of the incident beam. In addition, the existence of a lateral wave might prove useful for investigating crystal surfaces.

In this paper we will demonstrate that lateral shifts, lateral waves, and beam distortions do indeed result when a bounded x-ray beam is dynamically Bragg reflected from crystal planes. A few special cases have already been studied—namely, the shape of the reflected beam when an infinitely narrow (δ function) incident beam is Bragg reflected[7] and the lateral shift of a finite-width beam which undergoes symmetric reflection.[8] Here, we present a more general situation which includes the possibility of asymmetric as well as symmetric reflection and we will derive analytic expressions for the lateral shift for incidence both within and at the edges of the range of total reflection.

Because this analysis uses the language and results of the dynamical theory of x-ray diffraction, we will summarize the pertinent results of this theory in Sec. II. In Sec. III we will extend the usual plane-wave results in order to account for an incident bounded beam. In Secs. IV and V we will consider several specific examples to illustrate the shape and position of the reflected beam.

II. PLANE-WAVE DYNAMICAL X-RAY DIFFRACTION: A SUMMARY

Reviews of the dynamical theory of x-ray diffraction can be found in Refs. 9–11. In the usual theory, when a plane wave with wave vector $\mathbf{k}_0$ is incident from the vacuum onto a crystal surface near the Bragg angle, it excites within the crystal a forward diffracted wave with wave vector $\mathbf{K}_0$ and a reflected wave of wave vector $\mathbf{K}_H$. These wave vectors are related by Bragg's law so that

$$\mathbf{K}_H=\mathbf{K}_0+\mathbf{H} , \quad (1)$$

where $\mathbf{H}$ is a reciprocal lattice vector. Because the crystal index of refraction differs only slightly from unity, $\mathbf{K}_0$ differs only slightly from $\mathbf{k}_0$. Similarly, the reflected wave in the vacuum has a wave vector $\mathbf{k}_H$ which differs only slightly from $\mathbf{K}_H$. Boundary conditions require that the components of the wave vector along the surface (say the x direction) be continuous so that $K_{0x}=K_{0x}$ and $K_{Hx}=k_{Hx}$. Figure 2 illustrates these vectors.

We will use the notation of Ref. 9, and, for simplicity, will consider the case of no absorption. The ratio of reflected to incident amplitudes can be written as a function of incident angle θ^i as

$$R(\theta^i)=\frac{|b|^{1/2}|P|\exp(i\nu)}{P} , \quad (2)$$

where

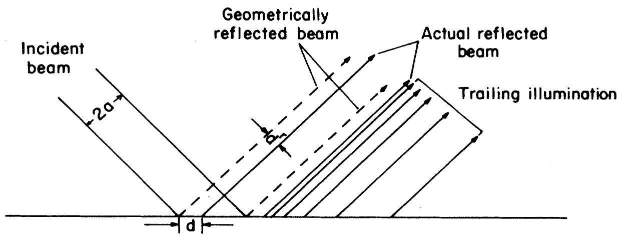

FIG. 1. Schematic representation of the lateral shift and trailing illumination for total internal reflection of optical beams.

$$\nu=\begin{cases}\pi+i\cosh^{-1}y, & y>1\\ \pi/2+\sin^{-1}y, & -1<y<1\\ i\cosh^{-1}-y, & y<-1\end{cases} \tag{3}$$

and

$$y=\frac{b(\theta^i-\theta_B)\sin(2\theta_B)+\Gamma F_0(1-b)/2}{\Gamma|P|\,|F_H|\,|b|^{1/2}} . \tag{4}$$

In Eqs. (2) and (4), P equals 1 for σ polarization and equals $\cos 2\theta_B$ for π polarization; F_H is the structure factor; $\Gamma=r_e\lambda/\pi V$; θ_B is the kinematic Bragg angle; and $b=-\sin\theta^i/\sin\theta^r$. For asymmetric Bragg diffraction, illustrated in Fig. 2, the scattering planes are not parallel to the surface. In this case, $\sin\theta^i\neq\sin\theta^r$ and $b\neq-1$. ($b=-1$ for symmetric Bragg diffraction.) In this paper we will specifically consider asymmetric diffraction but we will not consider extreme asymmetry for which θ^i or θ^r is very small (less than 10^{-2} rad). The approximations leading to Eqs. (2)–(4) are not valid in these extreme cases[12,13] and, in addition, grazing incidence results in a specularly reflected as well as a diffracted wave. This and other three wave problems are the subject of recent investigations,[14–18] and a study of lateral shifts for these situations will be considered in a later paper.

III. DIFFRACTION OF BOUNDED BEAMS

The physics of bounded beams has been described in Refs. 2–6. In particular, much of what follows for Bragg diffraction closely parallels the work of Horowitz and Tamir[2] and Tamir and Bertoni[3] for optical reflection. Consider a bounded beam incident on the crystal surface as is illustrated in Fig. 3 for a beam which has a Gaussian

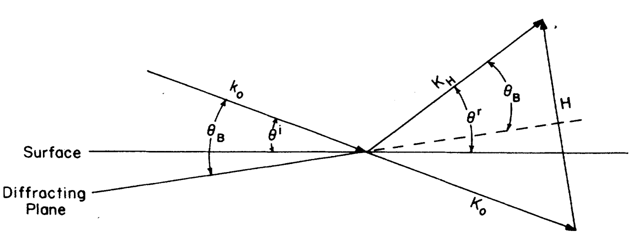

FIG. 2. Wave-vector geometry for asymmetric Bragg reflection.

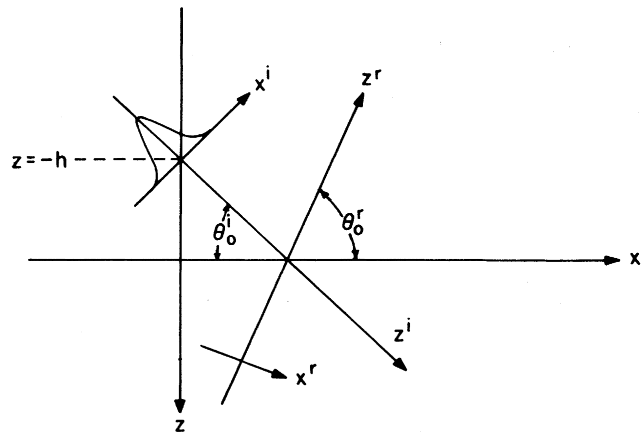

FIG. 3. Geometry and coordinate systems for asymmetric reflection of a bounded beam with a Gaussian cross section at $z=-h$. The origin of the reflected axes is at $x=h[\sin^2(\theta_0^r)\cot\theta_0^i-\sin(\theta_0^i)\cos\theta_0^r]$, $z=h\sin(\theta_0^r)[\cot(\theta_0^i)\cos\theta_0^r+\sin\theta_0^i]$.

cross section at $z^i=0$. This beam is directed at θ_0^i but, as we will demonstrate, consists of plane waves incident at angles θ^i which may differ slightly from θ_0^i. As indicated in Fig. 3, there are three coordinate systems of interest—the crystal coordinates (x,z), incident coordinates (x^i,z^i), and reflected coordinates (x^r,z^r). The incident and crystal coordinates are related by

$$\begin{aligned} x^i&=x\sin\theta_0^i-(h+z)\cos\theta_0^i ,\\ z^i&=x\cos\theta_0^i+(h+z)\sin\theta_0^i . \end{aligned} \tag{5}$$

If at $z^i=0$ the electric field varies across the beam as $F(x^i)$, then parallel to the crystal surface, at $z=-h$, this distribution is given by

$$\begin{aligned} E^i(x,-h)&=F(x^i)\exp(-ikz^i)|_{z=-h}\\ &=F(x\sin\theta_0^i)\exp(-ikx\cos\theta_0^i) . \end{aligned} \tag{6}$$

This field can be written as a Fourier sum of plane waves as follows:

$$E^i(x,-h)=\frac{1}{2\pi}\int_{-\infty}^{\infty}\Phi(\xi^i)\exp(-i\xi^i x)d\xi , \tag{7}$$

where

$$\begin{aligned} \Phi(\xi^i)&=\int_{-\infty}^{\infty}E^i(x,-h)\exp(i\xi^i x)dx\\ &=\int_{-\infty}^{\infty}F(x\sin\theta_0^i)\exp[i(\xi^i-\xi_0^i)x]dx , \end{aligned} \tag{8}$$

$$\xi^i=k\cos\theta^i \tag{9}$$

and

$$\xi_0^i=k\cos\theta_0^i . \tag{10}$$

For example, for a Gaussian distribution,

$$F(x^i)=\frac{\exp[-(x^i/a)^2]}{\sqrt{\pi}a} \tag{11}$$

and

$$\Phi(\xi^i)=\frac{\exp[-a(\xi^i-\xi_0^i)/2\sin\theta_0^i]^2}{\sin\theta_0^i} . \quad (12)$$

In general, at the crystal surface the incident beam is described by

$$E^i(x,0)=\frac{1}{2\pi}\int_{-\infty}^{\infty}\Phi(\xi^i)\exp[-i(\xi^i x+\alpha^i h)]d\xi^i , \quad (13)$$

where

$$\alpha^i=[k^2-(\xi^i)^2]^{1/2} . \quad (14)$$

Thus, at the surface, the incident beam is a sum of plane waves having spectral amplitude

$$\Phi(\xi^i)\exp(-i\alpha^i h) ,$$

which are incident at slightly different angles θ^i. Each incident wave excites a point on one of the dispersion surfaces giving rise to a Bragg reflected wave of amplitude

$$R(\theta^i)\Phi(\xi^i)\exp(-i\alpha^i h) ,$$

which propagates at angle θ^r. The resultant reflected beam, directed at angle θ_0^r, is a superposition of these reflected waves and can be written as

$$E^r(x,z)=\frac{1}{2\pi}\int_{-\infty}^{\infty}R(\theta^i)\Phi(\xi^i) \times\exp(-i\alpha^i h)\exp[-i(\xi^r x-\alpha^r z)]d\xi^i . \quad (15)$$

We note that $\Phi(\xi)$ approaches zero for $(\theta^i-\theta_0^i)>1/ak$ so that only values of θ close to θ_0 contribute to the integrand. Hence, $(\theta-\theta_0)\ll 1$ and we can write

$$(\xi-\xi_0)=k(\cos\theta-\cos\theta_0)=-k\sin\theta_0(\theta-\theta_0) \quad (16)$$

and

$$(\alpha-\alpha_0)=k\cos\theta_0(\theta-\theta_0)=-\cot\theta_0(\xi-\xi_0) . \quad (17)$$

In addition, as discussed in Sec. II, boundary conditions require that the x components of the forward and reflected wave vectors be continuous so that the x component of Eq. (1) can be written as

$$K_{Hx}=k_{0x}+H_x , \quad (18)$$

so that

$$k\cos\theta^r=k\cos\theta^i+H_x$$

and

$$k\cos\theta_0^r=k\cos\theta_0^i+H_x \quad (19)$$

and

$$(\xi^r-\xi_0^r)=(\xi^i-\xi_0^i) .$$

The reflected coordinates are related to the crystal coordinates by

$$x^r=x\sin\theta_0^r+z\cos\theta_0^r-h\cot\theta_0^i\sin\theta_0^r ,$$
$$z^r=x\cos\theta_0^r-z\sin\theta_0^r+h\sin\theta_0^i . \quad (20)$$

so that using Eqs. (16), (17), (19), and (20), Eq. (15) can be rewritten as

$$E^r(x,z)=\exp(-ikz^r)\frac{1}{2\pi} \times\int_{-\infty}^{\infty}R(\theta^i)\Phi(\xi^i)\exp\left[\frac{-i(\xi^i-\xi_0^i)x^r}{\sin\theta_0^r}\right]d\xi^i . \quad (21)$$

Note that the origin of the reflected coordinate system is chosen so that a geometric reflection $[R(\theta)=1]$ will propagate in direction z^r.

In order to simplify later calculations, we write

$$R(\theta^i)=\frac{|b|^{1/2}|P|}{P}\exp(i\nu_0)\exp[i(\nu-\nu_0)] , \quad (22)$$

and introduce

$$\sigma=y-y_0=-\frac{(\theta^i-\theta_0^i)}{2\Psi_B} , \quad (23)$$

where Ψ_B, the angular half-width for Bragg reflection, is defined as

$$\Psi_B=\frac{\Gamma F_H|P|}{|b|^{1/2}\sin(2\theta_B)} . \quad (24)$$

We will also write

$$\sigma=\Delta(\xi-\xi_0) , \quad (25)$$

and define

$$\Delta=\frac{|b|^{1/2}\sin(2\theta_B)}{k\Gamma F_H|P|\sin\theta_0^i}=\frac{|b|^{1/2}\sin\theta_B}{\sin\theta_0^i}\Delta_s . \quad (26)$$

Δ_s is the symmetric value of Δ appropriate for $b=-1$ and $\theta_0^i=\theta_0^r=\theta_B$.

In this new notation we can rewrite Eq. (21) as

$$E^r(x,z)=\frac{|b|^{1/2}|P|}{2\pi P}\exp(i\nu_0)\exp(-ikz^r)\int_{-\infty}^{\infty}\exp[i(\nu-\nu_0)]\Phi\left[\frac{\sigma}{\Delta}\right]\exp\left[\frac{-i\sigma x^r}{\Delta\sin\theta_0^r}\right]\frac{d\sigma}{\Delta} , \quad (27)$$

where $\Phi(\sigma/\Delta)$ is obtained by substituting Eq. (25) into Eq. (12). Although the integral in Eq. (27) can always be computed numerically, it can also be evaluated analytically for particular forms of Φ for certain approximations. Thus, for relatively wide beams ($a\gg\Delta$), the spectral distribution is narrow, and although, in principle, the integral in Eq. (27) must be evaluated from $-\infty$ to $+\infty$, only those values of σ for which $|\sigma|\ll 1$ play an important part in the integrand. As we will demonstrate in Secs. IV and V, the shape and displacement of the resultant reflected beam will be qualitatively different for spectrally narrow and spectrally wide incident beams. We also note from Eq. (23) that $|\sigma| \ll 1$ indicates that the angular spread of the incident beam is much less than the angular width for Bragg reflection. For asymmetric diffraction with $|b| < 1$ (small incident angle), Ψ_B is larger than for symmetric diffraction. Thus, beams which may be considered spectrally wide for the symmetric case are narrower for asymmetric scattering. Similarly, for $|b| > 1$, beams are now spectrally wider.

IV. SPECTRALLY NARROW INCIDENT BEAMS

We will first consider a spectrally narrow beam ($|\sigma| \ll 1$) which is incident within the range of total reflection ($-1 < y_0 < 1$). In this approximation, using Eq. (3), we have

$$\begin{aligned}\nu-\nu_0 &= \sin^{-1}y-\sin^{-1}y_0\\ &= \sin^{-1}[y(1-y_0^2)^{1/2}-y_0(1-y^2)^{1/2}]\\ &\approx (y_0+\sigma)(1-y_0^2)^{1/2}-y_0(1-y_0^2-2\sigma y_0)^{1/2} . \end{aligned} \tag{28}$$

If $\sigma y_0/(1-y_0{}^2) \ll 1$, then, expanding the last square root in Eq. (28), we find

$$\nu-\nu_0 \approx \frac{\sigma}{(1-y_0^2)^{1/2}} , \tag{29}$$

or

$$\nu-\nu_0 \approx \left.\frac{d\nu}{dy}\right|_{y=y_0}(y-y_0) . \tag{30}$$

Equation (30) is typically employed when evaluating $(\nu-\nu_0)$—both in the optical[5] and x-ray-diffraction[8] cases. That is, the phase of the reflection is usually expanded in powers of $(y-y_0)$, including up to linear terms. However, we see that $d\nu/dy$ is undefined for $y_0=\pm 1$ and, therefore, incidence at the edges of the range of total reflection must be treated separately. [Even if we were to include absorption, ν changes too rapidly at the edges to expand it in powers of $(y-y_0)$.] This is analagous to incidence at the critical angle for the optical Goos-Hanchen effect.[2] By substituting $y_0=\pm 1$ into Eq. (28) we see that at the edges of reflection

$$\nu-\nu_0 \approx -y_0\sqrt{-2\sigma y_0} . \tag{31}$$

A. Incidence within the range of total reflection

For a Gaussian beam incident within the reflecting range (away from the edges) we show in the Appendix that

$$E^r(x,z)=\frac{|P|\exp(i\nu_0)\exp(-ikz^r)}{|b|^{1/2}P}\,\frac{\exp\left[-\left\{\dfrac{x^r-\Delta\sin\theta_0^r/(1-y_0^2)^{1/2}}{a^r}\right\}^2\right]}{\sqrt{\pi}\,a^r} . \tag{32}$$

Thus, the reflected beam travels in the z^r direction with a Gaussian cross section which has half-width $a^r=a/|b|$ and which is centered not at $x^r=0$ but is shifted along x^r by

$$d^r=\frac{\Delta\sin\theta_0^r}{(1-y_0^2)^{1/2}} . \tag{33}$$

This corresponds to a lateral shift along the surface given by

$$d=\frac{\Delta}{(1-y_0^2)^{1/2}} . \tag{34}$$

We can compare the results for asymmetric versus symmetric diffraction by writing the symmetric displacement, d_s, as

$$d_s=\frac{\Delta_s}{(1-y_0^2)^{1/2}} , \tag{35}$$

and then rewriting Eq. (34) as

$$d=\frac{|b|^{1/2}\sin\theta_B}{\sin\theta_0^i}d_s . \tag{36}$$

Alternatively, we can compare the shift d^r to the reflected beam width a^r, for symmetric and asymmetric diffraction and we see that

$$\frac{d^r}{a^r}=|b|^{1/2}\frac{d_s^r}{a} . \tag{37}$$

The symmetric case has already been considered by Andreev[8] who obtained Eq. (35) and who calculated the shift as $d_s=56.8\ \mu\text{m}$ for $y_0=0$ for σ polarized Ag $K\alpha$ radiation ($\lambda=0.558$ Å) at the (555) reflection in silicon ($\theta_B=26.4^0$; $\Gamma F_H=0.28\times 10^{-6}$). From Eq. (37) we see that this shift can be enhanced for $|b|>1$. In addition, since Δ varies inversely as P, π polarized beams undergo larger displacements than σ polarized beams and multiple reflections of unpolarized beams can result in a separation of the polarizations. We also note from Eqs. (32) and (33) that this shift is independent of beam parameters. That is, it is independent of the exact shape of the incident beam.

B. Incidence at the edges of the reflecting range

The details of the evaluation of Eq. (27) for $y_0=\pm 1$ are carried out in the Appendix. Most importantly, we see from Eq. (A7) that $E^r(x,z)$ takes the form

$$E^r(x,z)=E_1(x,z)+E_2(x,z) , \tag{38}$$

where

$$E_1 = \frac{|b|^{1/2}|P|\exp(-ikz^r)\exp\left[-\left[\frac{x^r}{a^r}\right]^2\right]}{\sqrt{\pi}P|b|a^r} \tag{39}$$

and

$$E_2 = E_1\delta\ , \tag{40}$$

for

$$\delta = \frac{2^{1/4}\exp(3\pi i/4)(2\Delta\sin\theta_0^i)^{1/2}\exp\left[\frac{1}{2}\left[\frac{x^r}{a^r}\right]^2\right]D_{1/2}\left[-\frac{\sqrt{2}x^r}{a^r}\right]}{a^{1/2}}\ , \tag{41}$$

where $D_{1/2}$ is a parabolic-cylinder function.

We see that E_1 is a Gaussian beam traveling in the z^r direction with its axis along $x_r=0$. That is, it is the undistorted, unshifted reflection one would expect if the incident beam consisted of waves which were all incident at exactly θ_0^i. E_2 is due to the finiteness of the beam width which introduces waves at angles different from θ_0^i. For optical reflections, E_1 is termed the geometric reflection and E_2 is the lateral wave which, as we shall see below, interferes with E_1 for x^r near the beam axis, $x^r \ll a^r$, resulting in a lateral shift. For larger values of x^r, $x^r \gg a^r$, E_2 propagates along the surface and produces a "trailing illumination" parallel to E_1.

More specifically, we see from Eqs. (A18) and (A19) of the Appendix that for $x^r \ll a^r$

$$E^r = \frac{|b|^{1/2}|P|\exp(-ikz^r)\exp\left[-\left[\frac{x^r}{a^r}\right]^2+\delta'(0)\left[\frac{x^r}{a^r}\right]\right]}{\sqrt{\pi}P|b|a^r}$$
$$= \frac{|b|^{1/2}|P|\exp(-ikz^r)\exp[\delta'(0)/2]^2}{\sqrt{\pi}P|b|a^r}\exp-\left[\frac{(x^r-a^r\delta'(0)/2)}{a^r}\right]^2\ , \tag{42}$$

where

$$\delta'(0) = \frac{-\exp(3\pi i/4)(\Delta\pi\sin\theta_0^i)^{1/2}}{\sqrt{a}\,\Gamma(\frac{3}{4})}\ . \tag{43}$$

Thus, for $x^r \ll a^r$, the reflected beam propagates in the z^r direction with a Gaussian cross section which is shifted along x^r by

$$d^r = a^r\mathrm{Re}[\delta'(0)/2]$$
$$= \frac{(\cos\pi/4)(\Delta\pi a\sin\theta_0^i)^{1/2}}{2|b|\Gamma(\frac{3}{4})}\ , \tag{44}$$

producing a relative shift

$$\frac{d^r}{a^r} = \frac{(\cos\pi/4)(\Delta\pi\sin\theta_0^i)^{1/2}}{2\Gamma(\frac{3}{4})\sqrt{a}}\ . \tag{45}$$

We see that the shift at $y_0=\pm1$ is dependent on the incident beam width a, just as is the case for the optical shift for incidence at the critical angle.

For a beam of width $a=10^{-3}$ m, the shift for $y_0=\pm1$ is about three times larger than the shift for $y_0=0$. From Eq. (45) it appears that narrower incident beams undergo larger shifts relative to the beam width. However, very small values of a will invalidate the assumption that $\sigma \ll 1$ which lead to Eq. (45). Narrow beams are spectrally wide and will be discussed in Sec. V.

C. The lateral wave

We will now consider values of x^r such that $|x^r| \gg a^r$. For these large values of x^r, E_1 is essentially zero and the only contribution to E^r is from E_2. From Eqs. (A20) and (A22) of the Appendix, we see that for $x^r<0$, $E_2=0$ but for $x^r>0$, E_2 is approximated by

$$E_2 = \frac{|P|\exp(-ikz^r-i\pi/4)(\Delta\sin\theta_0^i)^{1/2}}{|b|\sqrt{\pi}P(x^r)^{3/2}}\ . \tag{46}$$

Thus, E_2 is a lateral wave which decays along the surface as $x^{-3/2}$ and produces a trailing illumination parallel to the z^r axis. This is analagous to optical reflection at the critical angle which is illustrated schematically in Fig. 1.

V. SPECTRALLY WIDE INCIDENT BEAMS

For spectrally wide beams we cannot make the approximations of Eqs. (28)–(31). Equation (27) has been evaluated numerically and the resulting reflected beam has been found to be distorted and broadened. Figure 4 illustrates the reflected intensity for various values of y_0 for an incident beam which has a uniform cross section for which $a=4\Delta\sin\theta$, $|b|=1$ and $P=1$. The dashed line represents the incident beam and also an undistorted, unshifted reflected beam. Note that the distorted beam has been shifted by approximately $0.25(a/\sin\theta)$ and for $a=4\Delta\sin\theta$ this shift is approximately Δ.

For an extremely narrow incident beam ($a \ll \Delta$) and for $y_0=0$ and $b=-1$, we show in the third subsection of the Appendix that the reflected beam has the form

$$E^r = \frac{i|P|\exp(-ikz^r)}{P\Delta\sin\theta_0}\left[\frac{1}{\zeta}J_1(\zeta)\right]\ , \tag{47}$$

where

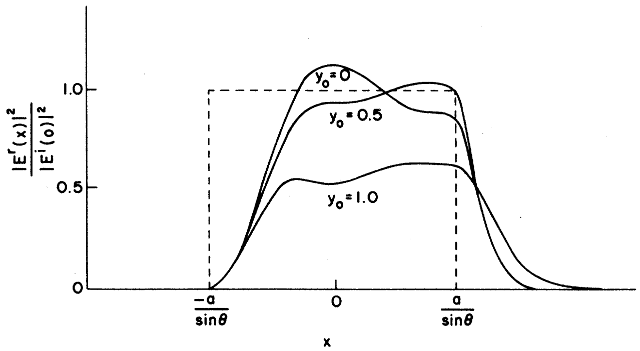

FIG. 4. Intensity of the reflected field along the crystal surface x for an incident beam of uniform intensity (dashed curve) for $a=4\Delta\sin\theta$.

$$\zeta=\frac{x^r}{\Delta\sin\theta_0^r}=\frac{x}{\Delta} \tag{48}$$

and J_1 is a Bessel function. Equation (47) agrees with the work of Uragami[7] who arrived at these results in a quite different manner—by integrating Takagi's equations[19] for an incident δ-function beam. Since the first zero of E^r is for $\zeta=1.22$, or $x=1.22\Delta$, the reflected beam is greatly broadened as compared to the incident beam although the peak of E^r is at $x=0$. (Since the geometrically reflected beam is of negligible width, interference between the geometrically reflected and lateral beams does not result in a lateral shift of the peak. However, due to the broadening, the beam centroid[8] is shifted.) For $x>1.22\ \Delta$, E^r exhibits subsidiary maxima or fringes, and using the asymptotic form of J_1 we see that for large x, E^r decays as $x^{-3/2}$, that is, it is a lateral wave.

VI. CONCLUSIONS

We have demonstrated that when a beam of x rays undergoes dynamical Bragg reflection, the reflected beam is displaced laterally along the crystal surface. The magnitude of this displacement depends on crystal parameters, x-ray wavelength and polarization, and the angular spread in the beam. We have shown that for spectrally narrow Gaussian beams the reflected beam is essentially undistorted and the lateral shift is enhanced for asymmetric diffraction. For incidence at the edge of the range of total reflection, where the phase of the reflected waves varies rapidly with angle, this shift is further enhanced and a lateral wave and trailing illumination are produced—similar to optical reflections for incidence at the critical angle. Finally, for spectrally wide beams, the reflection is distorted and broadened as well as shifted.

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APPENDIX: EVALUATION OF THE REFLECTED FIELD

We wish to evaluate Eq. (27) for a variety of situations, namely, for $a\gg\Delta(|\sigma|\ll 1)$ for both $y_0\neq\pm1$ and for $y_0=\pm1$ and also for $a/\Delta\ll 1$. In all cases we will assume an incident beam which has a Gaussian cross section as described in Eqs. (12) and (13).

1. Spectrally narrow beam incident within the range of reflection

For a Gaussian cross section, $|\sigma|\ll 1$ and $y_0\neq\pm1$, using Eq. (29) and defining

$$\Omega=\frac{\sigma}{\Delta\sin\theta_0^i}\ , \tag{A1}$$

Eq. (27) becomes

$$E^r(x,z)=\frac{|b|^{1/2}|P|}{2\pi P}\exp(i\nu_0-ikz^r)\int_{-\infty}^{\infty}\exp\left[-\frac{a^2}{4}\Omega^2-ib\Omega\left[x^r-\frac{\Delta\sin\theta_0^r}{(1-y_0^2)^{1/2}}\right]\right]d\Omega\ . \tag{A2}$$

This integral can be evaluated by completing the square or by using standard tables,[20] yielding

$$E^r(x,z)=\frac{|P|\exp(i\nu_0)\exp(-ikz^r)}{|b|^{1/2}P}\,\frac{\exp-\left[\dfrac{x^r-\Delta\sin\theta_0^r/(1-y_0^2)^{1/2}}{a^r}\right]^2}{\sqrt{\pi}\,a^r}\ , \tag{A3}$$

where

$$a^r=a/|b|\ . \tag{A4}$$

2. Spectrally narrow beam incident at the edge of reflection

When absorption is included, the reflection for $y_0=+1$ is different from that for $y_0=-1$. Neglecting absorption, however, the reflected beam is the same for both, and we, therefore, only give the details for $y_0=-1$. In this case, using Eq. (31), we have

$$\exp[i(\nu-\nu_0)]=\exp(i\sqrt{2\sigma})\ , \tag{A5}$$

and for $\sigma \ll 1$,

$$\exp[i(\nu-\nu_0)]=(1+i\sqrt{2\sigma}) . \quad \text{(A6)}$$

Thus, for incidence at the edge of reflection, Eq. (27) can be written as

$$E^r(x,z)=E_1(x,z)+E_2(x,z) , \quad \text{(A7)}$$

where

$$E_1=\frac{|b|^{1/2}|P|\exp(-ikz^r)}{2\pi P}\int_{-\infty}^{\infty}\exp(-a^2\Omega^2/4-i|b|x^r\Omega)d\Omega \quad \text{(A8)}$$

and

$$E_2=\frac{|b|^{1/2}|P|i(2\Delta\sin\theta_0^i)^{1/2}\exp(-ikz^r)}{2\pi P}\left[\int_0^{\infty}\Omega^{1/2}\exp(-a^2\Omega^2/4-i|b|x^r\Omega)d\Omega + i\int_0^{\infty}\Omega^{1/2}\exp(-a^2\Omega^2/4+i|b|x^r\Omega)d\Omega\right] . \quad \text{(A9)}$$

The integrals in Eqs. (A8) and (A9) are of standard form and when evaluated yield[21]

$$E_1=\frac{|b|^{1/2}|P|\exp(-ikz^r)\exp\left[-\left[\frac{x^r}{a^r}\right]^2\right]}{\sqrt{\pi}P|b|a^r} \quad \text{(A10)}$$

and

$$E_2=\frac{|b|^{1/2}|P|\exp(-ikz^r)i(2\Delta\sin\theta_0^i)^{1/2}}{2^{1/4}\pi P a^{3/4}}\Gamma(\tfrac{3}{4})\exp\left[-\frac{1}{2}\left[\frac{x^r}{a^r}\right]^2\right]\left[D_{-3/2}\left[\frac{-i\sqrt{2}x^r}{a^r}\right]+iD_{-3/2}\left[\frac{i\sqrt{2}x^r}{a^r}\right]\right] , \quad \text{(A11)}$$

where $D_p(q)$ is a parabolic-cylinder function. Noting that

$$D_p(q)=\frac{\Gamma(p+1)}{2\pi}[\exp(p\pi i/2)D_{-p-1}(iq)+\exp(-p\pi i/2)D_{-p-1}(-iq)] , \quad \text{(A12)}$$

we can rewrite E_2 as

$$E_2=E_1\delta , \quad \text{(A13)}$$

where

$$\delta=\frac{2^{1/4}\exp(3\pi i/4)(2\Delta\sin\theta_0^i)^{1/2}\exp\left[\frac{1}{2}\left[\frac{x^r}{a^r}\right]^2\right]D_{1/2}\left[-\frac{\sqrt{2}x^r}{a^r}\right]}{\sqrt{a}} . \quad \text{(A14)}$$

We will find it useful to evaluate E^r separately for points near the beam axis ($x^r \ll a^r$) and for points outside the beam width ($x^r \gg a^r$). In particular, for $x^r \ll a^r$ it is convenient to write

$$E^r=E_1\exp[\ln(1+\delta)] . \quad \text{(A15)}$$

We can then expand $\ln(1+\delta)$ in a power series in (x^r/a^r). Retaining up to linear terms we obtain

$$\ln(1+\delta)=\ln[1+\delta(0)]+\frac{\delta'(0)}{1+\delta(0)}\left[\frac{x^r}{a^r}\right] , \quad \text{(A16)}$$

where

$$\delta(0)=\frac{2\exp(3\pi i/4)(\Delta\pi\sin\theta_0^i)^{1/2}}{\sqrt{a}\,\Gamma(\frac{1}{4})} \quad \text{(A17)}$$

and

$$\delta'(0)=\frac{-\exp(3\pi i/4)(\Delta\pi\sin\theta_0^i)^{1/2}}{\sqrt{a}\,\Gamma(\frac{3}{4})} . \quad \text{(A18)}$$

For spectrally narrow beams, $\delta(0) \ll 1$, and we will approximate E^r as

$$E^r=\frac{|b|^{1/2}|P|\exp(-ikz^r)\exp\left[-\left[\frac{x^r}{a^r}\right]^2+\delta'(0)\left[\frac{x^r}{a^r}\right]\right]}{\sqrt{\pi}P|b|a^r}\ . \tag{A19}$$

For $|x^r|\gg a^r$ we can use the asymptotic (large argument) expansion of $D_{1/2}$ which is different for points to the left of the beam axis, $x^r<0$ and to the right, $x^r>0$.[22] For $x^r<0$,

$$D_{1/2}\left[\frac{-\sqrt{2}x^r}{a^r}\right]=\exp\left[-\frac{1}{2}\left[\frac{x^r}{a^r}\right]^2\right]\left[-\frac{\sqrt{2}x^r}{a^r}\right]^{1/2}, \tag{A20}$$

so that for large negative values of x^r we have $E_2=0$. For $x^r>0$,

$$D_{1/2}\left[\frac{-\sqrt{2}x^r}{a^r}\right]=\exp\left[-\frac{1}{2}\left[\frac{x^r}{a^r}\right]^2\right]\left[-\frac{\sqrt{2}x^r}{a^r}\right]^{1/2}-i\exp\left[\frac{1}{2}\left[\frac{x^r}{a^r}\right]^2\right]\frac{\sqrt{2\pi}}{\Gamma(-\frac{1}{2})}\left[-\frac{\sqrt{2}x^r}{a^r}\right]^{-3/2}, \tag{A21}$$

so that for large positive values of x^r we have

$$E_2=\frac{|P|\exp(-ikz^r-i\pi/4)(\Delta\sin\theta_0^i)^{1/2}}{|b|\sqrt{\pi}P(x^r)^{3/2}}\ . \tag{A22}$$

3. Spectrally wide incident beam

As an illustration of Bragg reflection of a spectrally wide beam, we will consider a particular example of a Gaussian beam for which $y_0=0$, $b=-1$, and $a/\Delta\ll 1$ (essentially a δ-function incident beam). We then have

$$\Phi(\xi)=1/\sin\theta_0\ . \tag{A23}$$

(Note that for $b=-1$, there is no need to differentiate between θ_0^i and θ_0^r.) We will rewrite Eq. (2) for $R(\theta)$ in an equivalent form as

$$\begin{aligned}R(\theta)&=-[y+(y^2-1)^{1/2}]\ ,\quad y<-1\ ,\\ R(\theta)&=-[y-i(1-y^2)^{1/2}]\ ,\quad -1\le y\le 1\ ,\\ R(\theta)&=-[y-(y^2-1)^{1/2}]\ ,\quad y>1\ .\end{aligned} \tag{A24}$$

Writing

$$\zeta=\frac{x^r}{\Delta\sin\theta_0^r}=\frac{x}{\Delta}\ , \tag{A25}$$

and noting that $\sigma=y$ for $y_0=0$, Eq. (21) now becomes

$$\begin{aligned}E^r&=-\frac{|P|\exp(-ikz^r)}{2\pi P\sin\theta_0}\left[\int_{-\infty}^{-1}[\sigma+(\sigma^2-1)^{1/2}]\exp(-i\sigma\zeta)\frac{d\sigma}{\Delta}+\int_{-1}^{1}[\sigma-i(1-\sigma^2)^{1/2}]\exp(-i\sigma\zeta)\frac{d\sigma}{\Delta}\right.\\ &\qquad\left.+\int_1^\infty[\sigma-(\sigma^2-1)^{1/2}]\exp(-i\sigma\zeta)\frac{d\sigma}{\Delta}\right]\\ &=\frac{i|P|\exp(-ikz^r)}{\pi P\Delta\sin\theta_0}\left[\int_0^\infty\sigma\sin(\sigma\zeta)d\sigma-\int_1^\infty(\sigma^2-1)^{1/2}\sin(\sigma\zeta)d\sigma+\int_0^1(1-\sigma^2)^{1/2}\cos(\sigma\zeta)d\sigma\right]\ .\end{aligned} \tag{A26}$$

If the first two integrals in Eq. (A26) are evaluated by expanding $\sin(\sigma\zeta)$ in powers of $\sigma\zeta$, it is clear that term by term they sum to zero. Using Ref. 23 we can evaluate the third integral so that

$$E^r=\frac{i|P|\exp(-ikz^r)}{P\Delta\sin\theta_0}\left[\frac{1}{\zeta}J_1(\zeta)\right], \tag{A27}$$

where J_1 is a Bessel function.

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[23]See Ref. 20, p. 419, Eq. (3.752-2).