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Relation of the Poynting vector normal to the dispersion surface

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Abstract. This communication is devoted to the so-called Ewald–Kato theorem, which declares that the Poynting vector is normal to the dispersion surface. Instead of the long-accepted hyperbolic result, an exact relation, valid for the whole of the Bragg-diffraction dispersion surface, is now pursued.

The dispersion surface is a useful concept in realizing Bragg diffraction of waves in periodic structures. Ewald (1958) and, more particularly, Kato (1958) have pointed out that the physical energy flow of waves in perfect crystals is normal to the dispersion surface. This geometric picture is similar to that for the case of visible rays and their relevant normal surface.

In the literature of the dynamical theory of diffraction, except for Kato's original proof, which gives a general consideration for the *N*-beam case (Chang, 1984), almost all authors [for example, James (1963) (§ 75 in particular) and Pinsker (1978)] express the readily proved relation between the Poynting vector and the dispersion surface by

$$\tan\Omega \simeq \left[\left(|v|^2-1\right)/\left(|v|^2+1\right)\right]\tan\theta_B, \quad (1)$$

considering only the 'hyperbolic' part of the dashed dispersion curve shown in Fig. 1(*a*). Note that Ω is the angle between the Poynting vector and the Bragg planes and v is the amplitude ratio of refracted waves given by (8) (see Appendix).

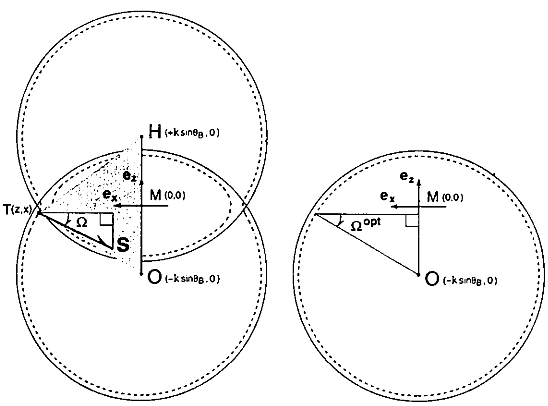
However, for the 'circular' part of the dashed curve, where $|v|$ is small, the slope of the normal to the dispersion curve comes close to

$$\tan\Omega^{\rm opt} = {\rm d}x/{\rm d}z = -(1/x)(z+k\sin\theta_B), \quad (2)$$

which is a total derivative of the optical refraction circle shown in Fig. 1(*b*); $n_O^2 = (z/k+\sin\theta_B)^2+(x/k)^2 = (1+\chi_O)$. For Fig. 1(*a*), (1) evidently fails in most parts of the dashed curve where Ω approaches $\Omega^{\rm opt}$ but $\Omega \neq -\theta_B$.

Because the theorem is generally established for Bragg diffraction, a rigorous proof for the two-beam case is very desirable. With the assumption of a *constant polarization factor*, which agrees with the case for σ-polarized X-rays as well as that for neutron diffraction (because the wave functions are scalar), an inverse of the tangent slope at any tie point T of (z,x),

$$\begin{aligned}{\rm d}x/{\rm d}z &= -(z/x)\Big\{\Big[z^2+x^2-k^2(1+\chi_O)-(k\sin\theta_B)^2\Big]\\ &\quad\times\Big[z^2+x^2-k^2(1+\chi_O)+(k\sin\theta_B)^2\Big]^{-1}\Big\},\end{aligned} \quad (3)$$



(*a*) (*b*)

Fig. 1. Excitation curve of X-rays in a crystal: (*a*) two-beam Bragg-diffraction dispersion surface cut in the zx plane, where $\mathbf{TO} = K_O = n_o k$, $\mathbf{TH} = K_H = n_H k$ and Ω is the angle between the Poynting vector S and the Bragg planes ($\parallel \hat{e}_x$); (*b*) one-beam Snell refraction circle, satisfied when $n_O = (1+\chi_O)^{1/2}$ = constant.

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is readily obtained from a total derivative of the fourth-order polynomial equation, (7), which is the exact expression of the dispersion curve.

The averaged Poynting vector, **S**, of each mode of waves excited in the crystal is proportional to $\mathbf{K}_O|E_O|^2+\mathbf{K}_H|E_H|^2$. So is its slope,

$$\begin{aligned}\tan\Omega &= \mathrm{Re}(\mathbf{S}\cdot\hat{\mathbf{e}}_z)/\mathrm{Re}(\mathbf{S}\cdot\hat{\mathbf{e}}_x)\\ &= -(1/x)\Big\{z+k\sin\theta_B\Big[\big(1-|v^2|\big)\\ &\quad\times\big(1+|v^2|\big)^{-1}\Big]\Big\}. \end{aligned} \tag{4}$$

We have $\tan\Omega = \mathrm{d}x/\mathrm{d}z$, because the right-hand sides of (3) and (4) can be shown to be identical and the relation of the Poynting vector normal to the dispersion surface for Bragg diffraction can then be derived. As the resonant region where z vanishes and $x \simeq k\cos\theta_B$ is approached, (4) approaches (1); away from the hyperbolic region, as $|v|$ becomes negligible, (4) gives the one-beam optical result of (2).

APPENDIX

In the general two-beam case, the fundamental wave-field equation gives the relation between the amplitudes of refracted waves *in* a crystal:

$$\begin{aligned}&\Big\{\chi_O+\big[\big(k^2-K_O^2\big)/k^2\big]\Big\}E_O+C^P\chi_{\bar{H}}E_H=0,\\ &C^P\chi_H E_O+\Big\{\chi_O+\big[\big(k^2-K_H^2\big)/k^2\big]\Big\}E_H=0,\end{aligned} \tag{5}$$

where χ_G $(G=O,H)$ is the Fourier component of the dielectric susceptibility and C^P $(P=\sigma,\pi)$ is the polarization factor. Recall that (5) is exact for the σ-polarized component ($C^\sigma = 1$) but is only approximate as the longitudinal part has been ignored for the π-polarized E_G field. For nontrivial solutions of E_O and E_H, refracted wave fields in the crystal, the secular equation gives

$$\begin{aligned}n_O^2 n_H^2 &= (1+\chi_O)\big(n_O^2+n_H^2\big)\\ &\quad-(1+\chi_O)^2+C^P\chi_H C^P\chi_{\bar{H}},\end{aligned} \tag{6}$$

where $n_G \equiv K_G/k$ is the refractive index. An orthogonal coordinate system is suggested in Fig. 1(*a*), with the origin M set at the center of **OH**, $\hat{\mathbf{e}}_z$ a unit vector of **OH** and $\hat{\mathbf{e}}_x$ parallel to the Bragg planes. Accordingly, the dashed locus (z,x) of tie points is well described by

$$\begin{aligned}&\Big[(z+k\sin\theta_B)^2+x^2\Big]\Big[(z-k\sin\theta_B)^2+x^2\Big]\\ &\quad=(1+\chi_O)\big[2\big(z^2+x^2+k^2\sin^2\theta_B\big)\big]\\ &\qquad-k^2(1+\chi_O)^2+k^2C^P\chi_H C^P\chi_{\bar{H}}.\end{aligned} \tag{7}$$

With a length parameter

$$Z \equiv -[(n_H^2-n_O^2)/2]/\big(C^P\chi_H C^P\chi_{\bar{H}}\big)^{1/2}$$

and eigenvalues solved from (6), we obtain the ratio of E_H to E_O as

$$\begin{aligned}v(i) &\equiv E_H(i)/E_O(i)\\ &= \Big[Z\pm\big(Z^2+1\big)^{1/2}\Big]\\ &\quad\times\big(C^P\chi_H C^P\chi_{\bar{H}}\big)^{1/2}/C^P\chi_{\bar{H}}\end{aligned} \tag{8}$$

from (5). Here, there are two modes; $i = 1$ for the plus-sign solution and $i = 2$ for the minus-sign solution.

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