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LETTER TO THE EDITOR

The relationship between the Poynting vector and the dispersion surface in the Bragg case

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Abstract. The relationship between the Poynting vector and the dispersion surface in the symmetrical Bragg case is studied in detail. It is found that the Poynting vector is not normal to the real part of the dispersion surface in the so-called 'total reflection' region, even when the contribution of the imaginary part of the scattering factor to the diffraction is negligible. Unlike that in the Laue case, the deviation in the Bragg case becomes least when the diffraction is induced only by the imaginary part of the scattering part near the absorption edge.

In our previous work [1], we found that, in the symmetrical Laue case, when the contribution of the imaginary part of the atomic scattering factor to the diffraction is comparable to that of the real part near the absorption edge, the direction Poynting vector within the crystal deviates from the normal of the real part of the complex dispersion surface. As we know, the diffraction and the dispersion surface in the Bragg case are quite different from those in the Laue case. So we address the question of whether the above-mentioned relationship is valid or not in the symmetrical Bragg case, which is the purpose of this letter. The notation is the same as in reference [1].

According to equation (22) in reference [1], the dispersion equation in the symmetrical Bragg case ($\beta = 0$) is as follows:

$$X^2 \cos^2\theta - Y^2 \sin^2\theta - 2\mathrm{i}\kappa_{0i} X \cos\theta - \kappa_{0i}^2 = \frac{P^2 \kappa_{0r}}{4} \chi_h \chi_{\bar{h}}. \tag{1}$$

The angle formed by the normal to the real part of the complex dispersion surface at the point (X, Y) and the X-axis is determined by the condition

$$\frac{\mathrm{d}x}{\mathrm{d}Y_1} = -\frac{(Y_1^2 + Y_2^2)\sin\theta}{\kappa_{0i} Y_2 - X Y_1 \cos\theta} \tan\theta \tag{2}$$

where Y_1 and Y_2 are the real and imaginary parts of Y, respectively.

As shown in figure 1, the direction of the averaged Poynting vector $\langle \boldsymbol{S} \rangle$ corresponding to the point (X, Y) is determined by the angle Δ. According to equations (10) and (25) in reference [1], we get

$$\tan\Delta = \frac{P_1}{-4XY_1 \sin\theta \cos\theta + 4Y_2 \kappa_{0i} \sin\theta} \tan\theta \tag{3a}$$

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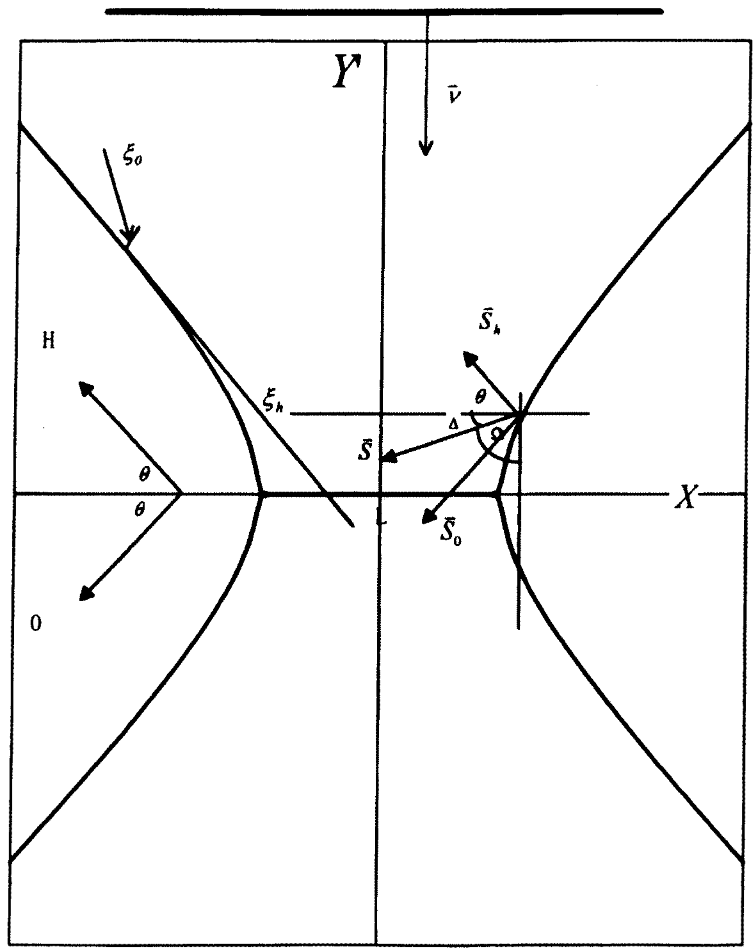

Figure 1. The Poynting vector and the real part of the dispersion surface in the symmetrical Bragg case.

and

$$P_1 = \{[(X\cos\theta - Y_1\sin\theta)^2 + (Y_2\sin\theta + \kappa_{0i})^2]^{1/2} - [(X\cos\theta + Y_1\sin\theta)^2 + (Y_2\sin\theta - \kappa_{0i})^2]^{1/2}\}^2. \quad (3b)$$

Following equation (1), we get

$$Y_1 = \frac{\kappa_{0r}|\bar{\chi}_h|}{2\sin\theta}\operatorname{Re}\sqrt{B} \quad (4a)$$

$$Y_2 = \frac{\kappa_{0r}|\bar{\chi}_h|}{2\sin\theta}\operatorname{Im}\sqrt{B} \quad (4b)$$

$$\operatorname{Re}\sqrt{B} = \left[\frac{1}{2}(C + B_1)\right]^{1/2} \quad (4c)$$

$$\operatorname{Im}\sqrt{B} = \pm\left[\frac{1}{2}(-C + B_1)\right]^{1/2} \quad (4d)$$

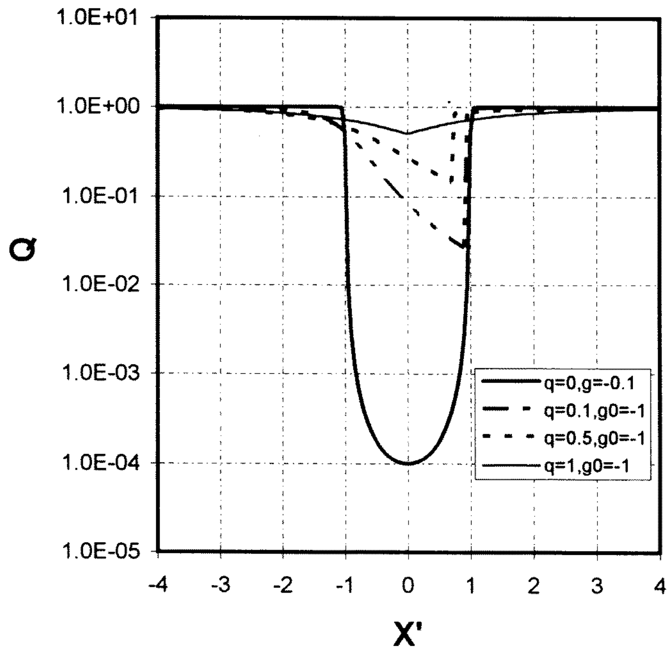

Figure 2. The variation of Q with respect to X for different cases in the symmetrical Bragg case.

$$B_1 = C^2 + D^2 \tag{4e}$$

$$C = X'^2 - g^2 - 1 + b^2 \tag{4f}$$

$$D = -2X'g - 2p\cos\delta \tag{4g}$$

$$X' = \frac{2\cos\theta}{\kappa_{0r}|\bar{\chi}_h|}X \tag{4h}$$

$$g = \frac{\chi_{0i}}{P|\bar{\chi}_h|} = g_0\sqrt{q}. \tag{4i}$$

In (4d), the sign '$-$' applies only when $D < 0$, since we deal with the Poynting vector pointing inward on the crystal. Combining equations (2), (3), and (4), we get

$$\frac{\mathrm{d}X}{\mathrm{d}Y_1} = -\frac{(\mathrm{Re}\sqrt{B})^2 + (\mathrm{Im}\sqrt{B})^2}{g\,\mathrm{Im}\sqrt{B} - X'\,\mathrm{Re}\sqrt{B}}\tan\theta \tag{5}$$

and

$$\tan\Delta = \frac{\{[(X' - \mathrm{Re}\sqrt{B})^2 + (\mathrm{Im}\sqrt{B} + g)^2]^{1/2} - [(X' + \mathrm{Re}\sqrt{B})^2 + (\mathrm{Im}\sqrt{B} - g)^2]^{1/2}\}^2}{-4X'\,\mathrm{Re}\sqrt{B} + 4g\,\mathrm{Im}\sqrt{B}} \times \tan\theta. \tag{6}$$

Using formulae (5) and (6), we can analyse the relationship between the direction of the Poynting vector and the dispersion surface in the symmetrical Bragg case. So we define the parameter Q as

$$Q = |\mathrm{d}X/\mathrm{d}Y_1|/|\tan\Delta|$$

$$= \frac{4[(\mathrm{Re}\sqrt{B})^2 + (\mathrm{Im}\sqrt{B})^2]}{\{\sqrt{(X' - \mathrm{Re}\sqrt{B})^2 + (\mathrm{Im}\sqrt{B} + g)^2} - \sqrt{(X' + \mathrm{Re}\sqrt{B})^2 + (\mathrm{Im}\sqrt{B} - g)^2}\}^2}. \quad (7)$$

As shown in figure 2, Q is calculated for different cases. When $q = 0$ and $g = -0.1$—which means that the contribution of the imaginary part of the atomic scattering factor to the diffraction is negligible for an absorbing crystal—we found that the Poynting vector deviates from the normal of the real part of the complex dispersion surface. The dispersion surface for this case is presented by Fukamachi *et al* [2]. As q increases, with the results that the contribution of the imaginary part becomes more and more comparable to that of the real part, the diffraction gradually decreases. When the diffraction is induced only by the imaginary part [3–7], the deviation is the least.

In the Bragg case, there are two fields corresponding to the two tie points in the dispersion surface in a plane-parallel crystal. The directions of their Poynting vectors are different, one toward the lower surface with a positive absorption coefficient, and the other toward the lower surface with a negative absorption coefficient. The former is much more important than the latter because the latter can be regarded as being produced by the former on the lower surface. Only by analysing the relationships between the Poynting vector and the dispersion surface in the Bragg case can we understand the negative effective absorption coefficient. The absorption coefficient along the Poynting vector is always positive. The calculation of this coefficient is usually based on the assumption that Poynting vectors are directed along the normals to the branches of the real part of the dispersion surface. However, we found that this assumption is not always valid. So the present results are very useful as regards the correct calculation of the absorption coefficient along the Poynting vector.

As pointed out in reference [7], the anomalous transmission takes place at the exact Bragg angle for a plane-parallel crystal in the Bragg case at which the contribution of the real part of the atomic scattering factor to the diffraction is smaller than that of the imaginary part. The explanation of the phenomenon needs the concept of a standing wave, which is strongly related to the Poynting vector and the dispersion surface. Since the transmitted beam mainly arises from the wave field with a Poynting vector directed toward the lower surface, the observation of the transmitted beam is an indirect observation of the Poynting vector directed toward the lower surface, which will be a subject of future work.

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