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Abstract. The relationship of the Poynting vector and the dispersion surface in the absorbing crystal is studied in detail. It is found that the long-accepted concept in which the physical energy flow of waves in the absorbing crystal is normal to the real part of the dispersion surface is not valid when the contribution of the imaginary part of the atomic scattering factor to the diffraction is comparable to that of the real part.

1. Introduction

The dispersion surface is a useful concept in describing the propagation of the waves in periodic structures. Ewald [1] and, more particularly, Kato [2] have pointed out that the physical energy flow of waves in perfect crystals, which is described in terms of the Poynting vector, is normal to the dispersion surface when there is no absorption. This geometric picture is similar to that for the case of visible rays and their relevant normal surface. Batterman and Cole [3] stated that the physical energy flow of waves in the absorbing crystal is normal to the real part of the dispersion surface when $|F_{hr}| \gg |F_{hi}|$, where F_{hr} and F_{hi} are the contributions of the real and the imaginary parts of the atomic scattering factor to the structure factor F_h (h is an abbreviation for the Miller indices $[hkl]$).

With x-rays from a tunable synchrotron radiation source, it is possible to select the ratio of F_{hr} and F_{hi}, and make $|F_{hr}| \leqslant |F_{hi}|$, or even $F_{hr} = 0$, near the absorption edge of a component atom in the crystal [4–15]. In 1995, Fukamachi *et al* found that the shape of the dispersion surface is strongly related to the ratio of F_{hr} and F_{hi} [13].

In this paper, we intend to analyse the relationship of the direction of the Poynting vector and the real part of the dispersion surface in the absorbing crystal, changing the ratio of F_{hr} and F_{hi}.

2. The dispersion surface and the Poynting vector

The Fourier coefficients of 4π times the complex polarizability of the crystal can be written as

$$\chi_h = \chi_{hr} + i\chi_{hi} \tag{1}$$

where

$$\chi_{hr} = |\chi_{hr}| \exp(i\alpha_{hr}) = -\frac{4\pi e^2}{V m \omega^2} F_{hr} \tag{2}$$

$$\chi_{hi} = |\chi_{hi}| \exp(i\alpha_{hi}) = -\frac{4\pi e^2}{V m \omega^2} F_{hi}. \tag{3}$$

In (2) and (3), V is the unit-cell volume, ω the x-ray frequency, m the electron mass and e the electron charge. The phase difference is given by

$$\delta = \alpha_{hi} - \alpha_{hr}. \tag{4}$$

The product of χ_h and $\chi_{\bar{h}}$ can be written as

$$\chi_h \chi_{\bar{h}} = |\bar{\chi}_h|^2 (1 - b^2 + i 2p \cos \delta) \tag{5}$$

where

$$|\bar{\chi}_h|^2 = |\chi_{hr}|^2 + |\chi_{hi}|^2 \tag{6}$$
$$b = \sqrt{2} |\chi_{hi}| / |\bar{\chi}_h| \tag{7}$$
$$p = |\chi_{hr}| |\chi_{hi}| / |\bar{\chi}_h|^2. \tag{8}$$

If we define the parameter

$$q = \frac{1}{1 + |\chi_{hr}/\chi_{hi}|^2}$$

then $b = \sqrt{2q}$, and $p = \sqrt{q(q-1)}$.

In the two-beam approximation [3, 16, 17, 18, 19], the displacement field within the crystal is a Bloch wave of the form

$$D = e^{-i\omega t}(D_0 e^{-i k_0 \cdot r} + D_h e^{-i k_h \cdot r}) \tag{9}$$

where $k_h = k_0 + h$ (h is the reciprocal vector) and the amplitude satisfy the system of equations

$$\begin{aligned}
2(\xi_0 - i\kappa_{0i})D_0 - P\chi_{\bar{h}}\kappa_{0r}D_h &= 0 \\
-P\chi_h\kappa_{0r}D_0 + 2(\xi_h - i\kappa_{0i})D_h &= 0
\end{aligned} \tag{10}$$

with the resonance defects ξ_0 and ξ_h defined by

$$\xi_0 = (k_0 \cdot k_0)^{1/2} - \kappa_{0r} \tag{11}$$
$$\xi_h = (k_h \cdot k_h)^{1/2} - \kappa_{0r} \tag{12}$$

where $\kappa_{0r} = K(1 + \frac{1}{2}\chi_{0r})$ and $\kappa_{0i} = K\chi_{0i}$, where K is the incident vacuum wavevector and P is the polarization factor. As the determinant of this system is zero,

$$(\xi_0 - i\kappa_{0i})(\xi_h - i\kappa_{0i}) = \kappa_{0r}^2 P^2 \chi_h \chi_{\bar{h}} \tag{13}$$

gives the equation of *a dispersion surface in reciprocal space*. This surface is a two-sheet surface of revolution (a hyperbolic cylinder) about the axis OH, where O and H are nodes of the reciprocal lattice; see figure 1.

With the tangential continuity boundary condition, the wavevectors in an absorbing crystal can be written as

$$k_0 = k_{0r} + i k_{0i} v \tag{14}$$
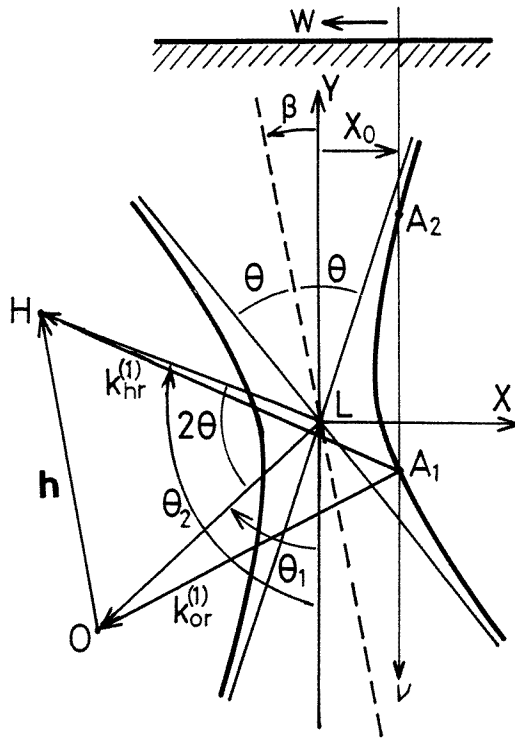$$k_h = k_0 + h = k_{hr} + i k_{0i} v \tag{15}$$

Figure 1. A schematic diagram of the dispersion surface. The origin of the reciprocal lattice is O, the diffracting point is H and the Laue point is L. Axis X is parallel to the crystal surface.

where v is a unit vector normal to the entrance surface and points inward, as shown in figure 1. Since $|k_{0r}| \gg |k_{0i}|$ and $|k_{hr}| \gg |k_{0i}|$ (this assumption being correct even when $|F_{hr}| \leqslant |F_{hi}|$), according to (11) and (13) we have

$$\xi_0 = |k_{0r}| - \kappa_{0r} + ik_{0i} \cos \theta_1 \tag{16}$$

$$\xi_h = |k_{hr}| - \kappa_{0r} + ik_{0i} \cos \theta_2. \tag{17}$$

It can be seen that the real parts of ξ_0 and ξ_h represent the distances between the tie points in the dispersion surface and the Laue spheres centred at the points O and H with a radius $R = \kappa_{0r}$, their imaginary parts being proportional to the absorption coefficients along the wavevectors.

In Batterman and Cole's treatment (p 696 in [3]), they made two additional assumptions: (1) $|F_{hr}| \gg |F_{hi}|$, and (2) $(|k_{hr}| - \kappa_{0r})(|k_{0r}| - \kappa_{0r}) \gg (k_{hi} \cos \theta_2 - \kappa_{0i})(k_{0i} \cos \theta_1 - \kappa_{0i})$. Under these assumptions, the real part of the dispersion surface is of the same shape as that when there is no absorption. In our treatment, we discard these assumptions, since the contribution of the imaginary part of the atomic scattering factor to the diffraction can be comparable to that of the real part near the absorption edge.

As shown in figure 1, X and the real part of Y represent the horizontal and vertical distances between the Laue point and the tie point, the imaginary part of Y being proportional to the absorption coefficients along v. The relationship between (ξ_0, ξ_h) and (X, Y) can be written as

$$\xi_0 = X \sin \theta_1 + Y \cos \theta_1 \tag{18}$$

$$\xi_h = X \sin \theta_2 + Y \cos \theta_2 \tag{19}$$

where

$$\theta_1 = \frac{\pi}{2} - \theta - \beta \tag{20}$$

$$\theta_2 = \frac{\pi}{2} + \theta - \beta. \tag{21}$$

θ is the Bragg angle, and β is the angle between the diffracting surface and the crystal surface. Substituting (18) and (19) into (13), we have

$$X^2 \sin \theta_1 \sin \theta_2 + Y^2 \cos \theta_1 \cos \theta_2 + XY \sin 2\beta - 2i\kappa_{0i} \cos \theta (X \cos \beta + Y \sin \beta) - \kappa_{0i}^2$$
$$= \frac{\kappa_{0r}^2 P^2}{4} \chi_h \chi_{\bar{h}}. \tag{22}$$

This is the dispersion equation in the rectangular coordinates X and Y. In the symmetrical Laue case, $\beta = \pi/2$, equation (22) can be simplified as

$$Y^2 \cos^2 \theta - X^2 \sin^2 \theta - 2i\kappa_{0i} Y \cos \theta - \kappa_{0i}^2 = \frac{\kappa_{0r}^2 P^2}{4} \chi_h \chi_{\bar{h}}. \tag{23}$$

The angle formed by the normal to the real part of the dispersion surface (17) at point (X, Y) with the X-axis is determined by the condition

$$\frac{dX}{dY_1} = \frac{(\kappa_{0i} - Y_2 \cos \theta)^2 + (Y_1 \cos \theta)^2}{Y_1 X \sin \theta \cos \theta} \cotan \theta \tag{24}$$

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

The averaged Poynting vector $\langle S \rangle$ corresponding to the point (X, Y) can be given by

$$\langle S \rangle = \frac{c}{8\pi} e^{4\pi k_i \cdot r} \left[|D_0|^2 \frac{k_0}{|k_0|} + |D_h|^2 \frac{k_h}{|k_h|} \right]. \tag{25}$$

As shown in figure 2, the direction of the vector $\langle S \rangle$ is determined by the angles Δ and Ω. It follows immediately from figure 2 that

$$\frac{\sin(\theta + \Delta)}{\sin(\theta - \Delta)} = \frac{|D_0|^2}{|D_h|^2}. \tag{26}$$

So we get

$$\tan \Delta = \frac{|D_0|^2 - |D_h|^2}{|D_0|^2 + |D_h|^2} \tan \theta. \tag{27}$$

Therefore,

$$\tan \Omega = \frac{|D_0|^2 + |D_h|^2}{|D_0|^2 - |D_h|^2} \tan \theta. \tag{28}$$
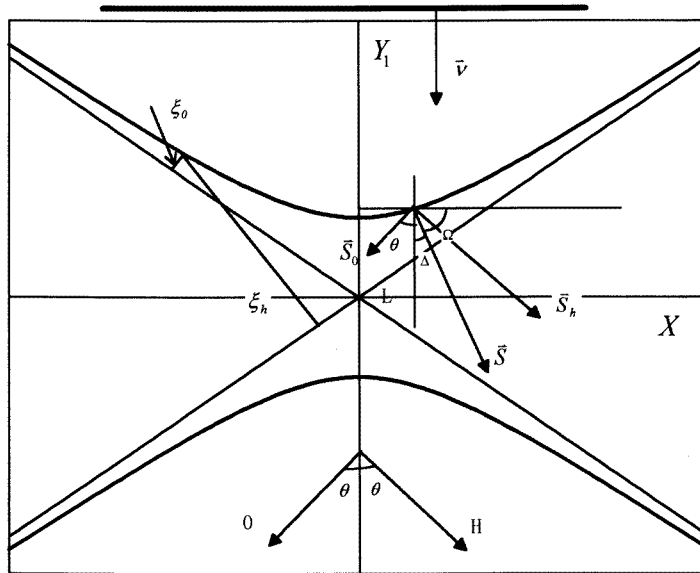
According to (10) and (28), we get

$$\tan \Omega = \left\{ \left[\sqrt{(Y_1 \cos \theta + X \sin \theta)^2 + (Y_2 \cos \theta - \kappa_{0i})^2} \right. \right.$$
$$\left. \left. + \sqrt{(Y_1 \cos \theta - X \sin \theta)^2 + (Y_2 \cos \theta - \kappa_{0i})^2} \right]^2 \middle/ [4Y_1 X \sin \theta \cos \theta] \right\}$$
$$\times \cotan \theta. \tag{29}$$

According to (23), we get

$$Y_1 \cos \theta = (\pm) \frac{\kappa_{0r} |\bar{\chi}_h|}{2} \mathrm{Re}[X'^2 + (1 - b^2 + i2p \cos \delta)]^{1/2} \tag{30}$$

$$\kappa_{0i} - Y_2 \cos \theta = (\pm) \frac{\kappa_{0r} |\bar{\chi}_h|}{2} \mathrm{Im}[X'^2 + (1 - b^2 + i2p \cos \delta)]^{1/2} \tag{31}$$

Figure 2. The relationship of the Poynting vector and the dispersion surface in the symmetrical Laue case when there is no absorption.

where the $\pm$ correspond to the two tie points in the dispersion surface, and X' is given by

$$X' = \frac{2\sin\theta}{\kappa_{0r}P|\bar{\chi}_h|}X. \tag{32}$$

Without loss of generality, it is enough to deal with one tie point. Equations (24) and (29) can be written as

$$\frac{\mathrm{d}X}{\mathrm{d}Y_1} = \frac{4\{[\mathrm{Im}\sqrt{L}]^2 + [\mathrm{Re}\sqrt{L}]^2\}}{4X'\,\mathrm{Re}\sqrt{L}}\cotan\theta \tag{33}$$

and

$$\tan\Omega = \frac{\left[\sqrt{(\mathrm{Re}\sqrt{L}+X')^2 + (\mathrm{Im}\sqrt{L})^2} + \sqrt{(\mathrm{Re}\sqrt{L}-X')^2 + (\mathrm{Im}\sqrt{L})^2}\right]^2}{4X'\,\mathrm{Re}\sqrt{L}}\cotan\theta \tag{34}$$

where

$$L = X'^2 + (1 - b^2 + \mathrm{i}\,2p\cos\delta) \tag{35}$$

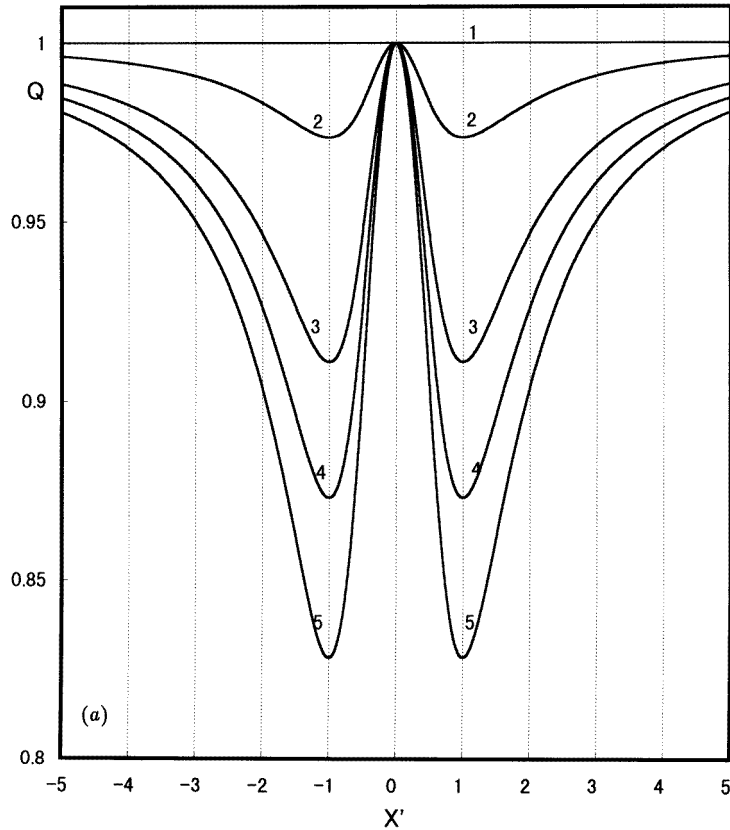$$\mathrm{Re}\sqrt{L} = \left[\frac{1}{2}(A + L_1)\right]^{1/2} \tag{36}$$

$$\mathrm{Im}\sqrt{L} = \left[\frac{1}{2}(-A + L_1)\right]^{1/2} \tag{37}$$

$$L_1 = (A^2 + B^2)^{1/2} \tag{38}$$

$$A = X'^2 + 1 - b^2 \tag{39}$$

$$B = 2p\cos\delta. \tag{40}$$

Using formulae (33) and (34), we can analyse the relationship between the direction of the Poynting vector and the dispersion surface.

Figure 3. The variation of Q with respect to X' for different values of q: (1): $q = 0$; (2): $q = 0.1$; (3): $q = 0.3$; (4): $q = 0.4$; (5): $q = 0.5$; (6): $q = 0.6$; (7): $q = 0.7$ (8): $q = 0.9$; (9): $q = 1$.

3. Discussion and conclusion

3.1. No absorption

In this case, $b = p = 0$, $\text{Re}\sqrt{L} = \sqrt{X'^2 + 1} > |X'|$, $\text{Im}\sqrt{L} = 0$,

$$\left| \frac{\mathrm{d}X}{\mathrm{d}Y_1} \right| = \frac{\sqrt{X'^2 + 1}}{|X'|} \cotan \theta = |\tan \Omega| \tag{41}$$

and the Poynting vector is perpendicular to the dispersion surface, which is consistent with the results of Kato and Ewald [1, 2].

3.2. With absorption

3.2.1. The case where $q \approx 0$ ($|\chi_{hi}| \ll |\chi_{hr}|$). This situation is usually regarded as taking place only when the energy of the incident x-ray is far from the absorption edge. However, Fukamachi *et al* found that it may take place when the energy of the incident x-ray is about 7 eV below the Ga K-absorption edge for the GaAs (200) quasi-forbidden reflection, and observed the phase change of the x-ray polarizability [9]. In this case, the parameters in
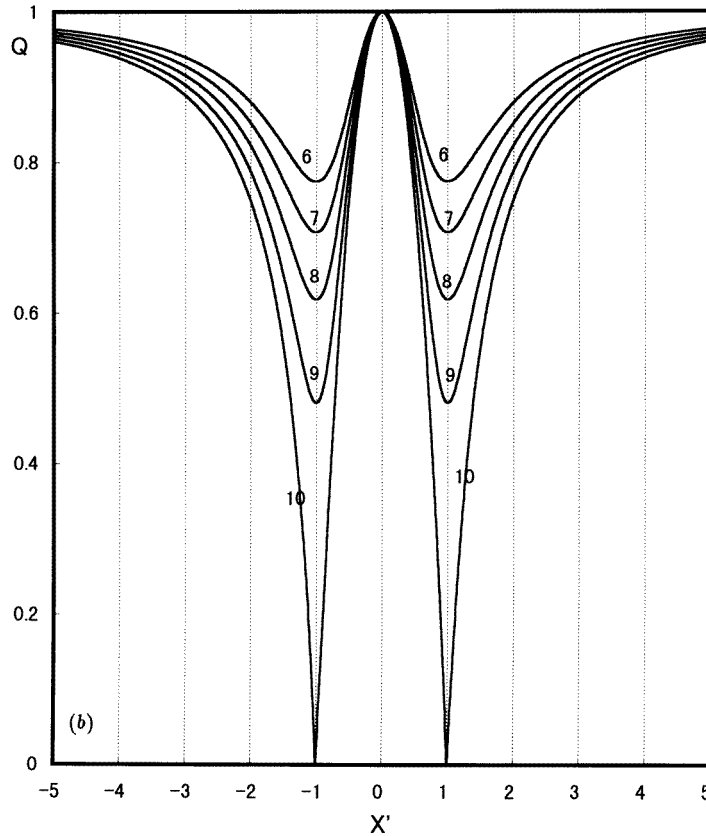
Figure 3. (Continued)

(24) and (25) are the same as those in the case of no absorption. The Poynting vector is perpendicular to the real part of the dispersion surface, which is consistent with the result of Batterman and Cole [3].

3.2.2. The case where $0 < q < 1$ ($\chi_{hr}\chi_{hi} \neq 0$). According to (33) and (34), when $X' = 0$ (at the exact Bragg angle), $|dX/dY_1| = |\tan \Omega| = \infty$, the energy flows along the diffracting lattice. When $X' \neq 0$, since the imaginary part of L is not zero, $\mathrm{Re}\sqrt{L} \neq 0$, it is enough to compare the value of Q with 1, where Q is given by

$$Q = \frac{|dX/dY_1|}{|\tan \Omega|} = \frac{4\{[\mathrm{Im}\sqrt{L}]^2 + [\mathrm{Re}\sqrt{L}]^2\}}{\left[\sqrt{(\mathrm{Re}\sqrt{L} + X')^2 + (\mathrm{Im}\sqrt{L})^2} + \sqrt{(\mathrm{Re}\sqrt{L} - X')^2 + (\mathrm{Im}\sqrt{L})^2}\right]^2}.$$

(42)

As shown in figure 3, Q is calculated for different values of q. It can be seen that when $0 < q < 1$, in the region where $X' \neq 0$, the value of Q is smaller than 1, which means that the Poynting vector gradually deviates from the normal of the real part of the dispersion surface. The deviation increases with increasing q. For a given q, the deviation is the largest when $|X'| = 1$. When $|X'| \to \infty$, $Q \to 1$, the deviation vanishes.
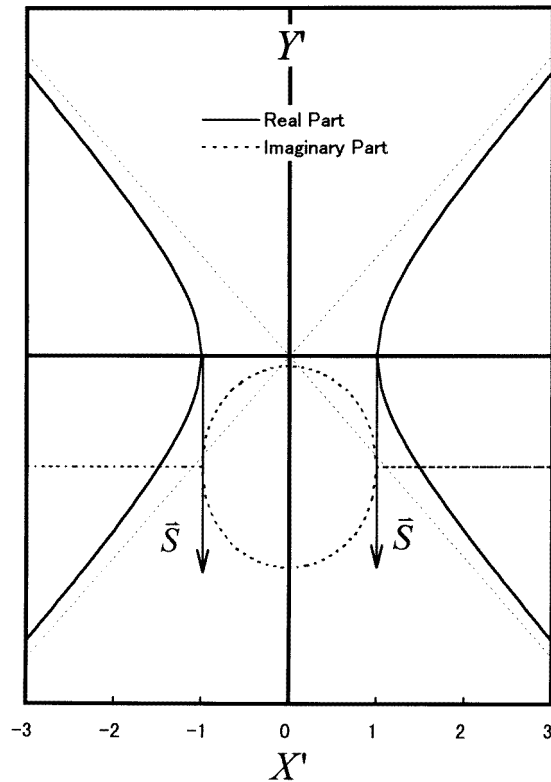
Figure 4. The complex dispersion surface when diffraction is induced only by the imaginary part of the atomic scattering factor. $Y' = [2\sin\theta/(\kappa_{0r}|\bar{\chi}_h|)]Y$. The Poynting vector is nearly tangential to the real part of the surface when $X' = \pm 1$.

3.2.3. The case where $q = 1$ ($\chi_{hr} = 0$). In this case, the diffraction is induced only by the imaginary part of the atomic scattering factor [8, 10, 12, 14, 15] and the dispersion surface in the symmetrical Laue case is similar to that in the symmetrical Bragg case with no absorption [14]. According to (35), $L = X'^2 - 1$, so in the region of $|X'| < 1$, $\text{Re}\sqrt{L} = 0$, $|dX/dY_1| = |\tan\Omega| = \infty$, the energy flows along the diffracting lattice. When $|X'| \approx 1$, the Poynting vector is nearly tangential to the real part of the dispersion surface, as shown in figure 4. In the region where $|X'| > 1$, $Q \neq 1$ (see figure 3(*b*)), the Poynting vector deviates from the normal of the real part of the dispersion surface.

Because of the anomalous absorption and penetration, the direction of the Poynting vector of the total fields in the crystal does not change with the distance from the crystal surface; it only changes when the two fields flow in the same direction. According to the above analysis and formulae (33) and (34), it can be seen that this condition is satisfied only at the exact Bragg angle if $q \neq 1$, which makes the energy flow very difficult to observe [20]. However, if $q = 1$, the two fields flow along the diffracting lattice in the region where $|X'| < 1$, which corresponds to a small-angle range deviating from the exact Bragg angle. This may be helpful in the experimental observation of the energy flow for an absorbing crystal.

Acknowledgments

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