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The Flow of X-rays and Material Waves in Ideally Perfect Single Crystals

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It is shown that in any wave field (X-rays, electrons, light) in a perfect crystal the direction of energy flow is along the normal of the surface of dispersion taken at the point of the surface representing the wave field. This holds for any polarization of the wave field and in particular under conditions where simultaneous reflections occur. This confirms the result obtained in a previous paper (Kato, 1952).

1. Introduction

Several years ago M. v. Laue showed the method for obtaining the energy flow of X-rays (1952), and more recently that of material particles (1953) in ideally perfect crystals. According to his calculation the Poynting vector $\boldsymbol{\gamma}$ (in the case of X-rays) and the current vector $\mathbf{T}$ (in the case of material particles) are very complicated on an atomic scale. But $\boldsymbol{\gamma}$ and $\mathbf{T}$ can be expressed by a comparatively simple form if they are averaged over time and space.

The present paper supplements his result by showing that the direction of these averaged vectors ($\overline{\overline{\boldsymbol{\gamma}}}$ and $\overline{\overline{\mathbf{T}}}$) is the same as the direction of the normal of the dispersion surface in the case of non-absorbing crystals. This relation is independent of simultaneous reflection and polarization. In addition, the relation holds also in crystal optics of visible rays.

In the following treatment we are only concerned with the case of X-ray diffraction because the case of material particles can be treated according to the same procedure.

2. Fundamental equations

According to the well known dynamical theory of X-rays (v. Laue, 1948; James, 1954) the wave fields $\mathbf{D}$ and $\mathbf{H}$ can be expressed by a Bloch function

$$\begin{aligned} \mathbf{D} &= \exp\,[j\nu t]\sum_m \mathbf{D}_m \exp\,[-j(\mathbf{k}_m\cdot\mathbf{r})] \\ \mathbf{H} &= \exp\,[j\nu t]\sum_m \mathbf{H}_m \exp\,[-j(\mathbf{k}_m\cdot\mathbf{r})]\,, \end{aligned} \tag{1}$$

where $\mathbf{k}_m$ are the wave vectors of diffracted beams and can be written as

$$\mathbf{k}_m = \mathbf{k}_0+\mathbf{b}_m\,. \tag{1'}$$

Here $\mathbf{k}_0$ is the wave vector of the primary beam and $\mathbf{b}_m$ are the reciprocal lattice vectors of the crystal. The amplitude of the component waves, $\mathbf{D}_m$ and $\mathbf{H}_m$, are determined by the following set of fundamental equations,

$$(\mathbf{k}^2-\mathbf{k}_m^2)\mathbf{D}_m = \sum_q \varphi_{m-q}(\mathbf{k}_m\times(\mathbf{k}_m\times\mathbf{D}_q)) \qquad (m=-\infty\ldots+\infty)\,, \tag{2}$$

where φ_n is the Fourier coefficient of the distribution of polarizability.

From these relations it is evident that every component wave is a transverse wave. Therefore it is sufficient to consider only two components $\mathbf{D}_{m\xi}$ and $\mathbf{D}_{m\eta}$. Here suffixes ξ and η indicate the mutually perpendicular directions of polarization. Multiplying equation (2) by the unit vectors $\mathbf{D}_{m\xi}/|\mathbf{D}_{m\xi}|$ and $\mathbf{D}_{m\eta}/|\mathbf{D}_{m\eta}|$ we obtain

$$\begin{aligned} \frac{\mathbf{k}^2-\mathbf{k}_m^2}{\mathbf{k}^2}D_{m\xi} &= -\sum_q\left\{\varphi\binom{qm}{\xi'\xi}D_{q\xi'}+\varphi\binom{qm}{\eta'\xi}D_{q\eta'}\right\} \\ \frac{\mathbf{k}^2-\mathbf{k}_m^2}{\mathbf{k}^2}D_{m\eta} &= -\sum_q\left\{\varphi\binom{qm}{\xi'\eta}D_{q\xi'}+\varphi\binom{qm}{\eta'\eta}D_{q\eta'}\right\}, \end{aligned} \tag{3}$$

where $\varphi\binom{qm}{\xi'\xi}$ etc. denote $\varphi_{m-q}\cos\chi_{mq;\,\xi\xi'}$, and $\chi_{mq;\,\xi\xi'}$ is the angle between $\mathbf{D}_{m\xi}$ and $\mathbf{D}_{q\xi'}$. The condition for (3) to have a non-trivial solution is

$$\left|\begin{array}{cccccc} \frac{\mathbf{k}^2-\mathbf{k}_m^2}{\mathbf{k}^2} & 0 & & & \varphi\binom{qm}{\xi'\xi} & \varphi\binom{qm}{\eta'\xi} \\ 0 & \frac{\mathbf{k}^2-\mathbf{k}_m^2}{\mathbf{k}^2} & & & \varphi\binom{qm}{\xi'\eta} & \varphi\binom{qm}{\eta'\eta} \\ & & \ddots & & & \\ \varphi\binom{mq}{\xi\xi'} & \varphi\binom{mq}{\eta\xi'} & & & \frac{\mathbf{k}^2-\mathbf{k}_q^2}{\mathbf{k}^2} & 0 \\ \varphi\binom{mq}{\xi\eta'} & \varphi\binom{mq}{\eta\eta'} & & & 0 & \frac{\mathbf{k}^2-\mathbf{k}_q^2}{\mathbf{k}^2} \end{array}\right| = 0\,. \tag{4}$$

Since $\mathbf{k}$ is considered given, this equation is, by virtue of (1'), an equation of infinite order for $\mathbf{k}_0$; it defines the dispersion surface in reciprocal space.

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We denote hereafter each branch of this equation and its relevant quantities by the superscript (α).

For a given $\mathbf{k}_0^{(\alpha)}$ which satisfies equation (4), the amplitude ratio of an arbitrary pair of two component waves can be determined as follows:

$$\frac{D_{m\xi}^{(\alpha)}}{D_{q\xi'}^{(\alpha)}} = \pm \frac{|m\xi;\ m\xi|^{(\alpha)}}{|q\xi';\ m\xi|^{(\alpha)}} \tag{5a}$$

or

$$\frac{D_{q\xi'}^{(\alpha)}}{D_{m\xi}^{(\alpha)}} = \pm \frac{|q\xi';\,q\xi'|^{(\alpha)}}{|m\xi;\,q\xi'|^{(\alpha)}} \tag{5b}$$

In these expressions, $|q\xi';\,m\xi|^{(\alpha)}$ means the small determinant derived from the original determinant, equation (4), by removing the $q\xi'$-column and the $m\xi$-row. Thus, if the amplitude of one component wave, say $D_{0\xi}^{(\alpha)}$, is given the amplitude of the other can be determined uniquely. The amplitude $D_{0\xi}^{(\alpha)}$ is determined by the boundary conditions of the wave field at the crystal surfaces.*

Inserting these component wave fields into equation (1) we obtain the total wave field as follows:

$$\begin{aligned}\mathbf{D} &= \exp\,[j\nu t] \sum_{\alpha}\sum_{m\xi} \mathbf{D}_{m\xi}^{(\alpha)} \exp\,[-j(\mathbf{k}_m^{(\alpha)}\cdot\mathbf{r})]\\ \mathbf{H} &= \exp\,[j\nu t] \sum_{\alpha}\sum_{m\xi} \mathbf{H}_{m\xi}^{(\alpha)} \exp\,[-j(\mathbf{k}_m^{(\alpha)}\cdot\mathbf{r})]\,.\end{aligned} \tag{1'}$$

3. Poynting vector and tangential plane of dispersion surface

According to Laue's treatment we obtain the averaged Poynting vector $\overline{\overline{\gamma}}$ as

$$\overline{\overline{\gamma}} = c/4\pi \sum_{\alpha}\sum_{\beta} \exp\,[-j(\mathbf{k}_0^{(\alpha)}-\mathbf{k}_0^{(\beta)}\cdot\mathbf{r}) \sum_{m\xi}\sum_{m\xi'} (\mathbf{D}_{m\xi}^{(\alpha)}\times\mathbf{H}_{m\xi'}^{(\beta)})\,. \tag{6}$$

In ordinary experimental conditions we observe a Poynting vector averaged over a region larger than a few microns, whereas the spatial periodicity of 'Pendellösung', $1/|\mathbf{k}_0^{(\alpha)}-\mathbf{k}_0^{(\beta)}|$, is of the same order of magnitude. Therefore it is sufficient to consider $\overline{\overline{\overline{\gamma}}}$ which means the vector $\overline{\overline{\gamma}}$ averaged over the period of Pendellösung. In addition there are the following relations

$$(\mathbf{D}_{m\xi}^{(\alpha)}\times\mathbf{H}_{m\xi'}^{(\alpha)}) = \begin{cases} \mathbf{k}_m^{(\alpha)}(D_{m\xi}^{(\alpha)})^2, & \xi' = \xi\\ 0, & \xi' = \eta\,. \end{cases} \tag{7}$$

Therefore

$$\overline{\overline{\overline{\gamma}}} = \sum_{\alpha} \gamma^{(\alpha)} \tag{8}$$

$$\gamma^{(\alpha)} = c/4\pi \sum_{m\xi} \mathbf{k}_m^{(\alpha)}(D_{m\xi}^{(\alpha)})^2\,. \tag{8'}$$

This result is essentially equivalent to Laue's result and shows that there exists a stream of energy $\gamma^{(\alpha)}$ corresponding to the α-branch of the dispersion surface and the total flow of energy can be expressed by the vector sum of all $\gamma^{(\alpha)}$.

Let us rewrite this equation in a more convenient form, using equations (5a) and (5b). Further, we omit the suffix (α) because we shall consider only $\gamma^{(\alpha)}$ hereafter. In the case of a non-absorbing crystal we have

$$\varphi_m = \varphi_{-m}^*\,.$$

The definition of $\chi_{q\xi';m\xi}$ gives

$$\chi_{q\xi';m\xi} = \chi_{m\xi;q\xi'}\,.$$

Thus it follows that

$$\varphi\binom{mq}{\xi\xi'} = \varphi^*\binom{qm}{\xi'\xi}\,. \tag{9}$$

This means that

$$|q\xi';\ m\xi| = |m\xi;\ q\xi'|^* \tag{10}$$

and in the special case

$$|m\xi;\ m\xi| = |m\xi;\ m\xi|^* = \text{real}. \tag{10'}$$

Therefore we find

$$\frac{|D_{m\xi}|^2}{|m\xi;\ m\xi|} = \frac{|D_{q\xi'}|^2}{|q\xi';\ q\xi'|} = \ldots = \text{const.}\dagger \tag{11}$$

Thus we can write the Poynting vector as follows

$$\gamma = c/(4\pi)\ \text{const.} \sum_{m\xi} \{\mathbf{k}_m|m\xi;\ m\xi|\}\,. \tag{12}$$

Next, we consider the tangential plane of the dispersion surface at a dispersion point D, i.e. $\overrightarrow{\mathbf{DO}} = \mathbf{k}_0$ and $\overrightarrow{\mathbf{DM}} = \mathbf{k}_m$. If we denote an infinitesimal vector on this contact plane by $\delta\boldsymbol{\tau}$, $\mathbf{k}_0+\delta\boldsymbol{\tau}$ also satisfies the equation of the dispersion surface. Therefore $\delta\boldsymbol{\tau}$ satisfies

$$\delta\,|\text{all}| = 0\,, \tag{13}$$

where $|\text{all}|$ denotes the determinant of the left side of equation (4), and δ operates on all $\mathbf{k}_m$.

Expanding $|\text{all}|$ by the elements of the $(m\xi)$-column and taking the variation, the left side of equation (13) is

$$\begin{aligned}&-2\mathbf{k}_m\delta\boldsymbol{\tau}|m\xi;\ m\xi| + \frac{\mathbf{k}^2-\mathbf{k}_m^2}{\mathbf{k}^2}\,\delta|m\xi;\ m\xi|\\ &\quad+\sum_{q\xi'}\varphi\begin{pmatrix}mq\\ \xi\xi'\end{pmatrix}\delta|m\xi;\ q\xi'|\\ &= -2\mathbf{k}_m\delta\boldsymbol{\tau}|m\xi;\ m\xi| + \delta_{m\xi}|\text{all}|\,,\end{aligned}$$

where $\delta_{m\xi}$ denotes the variational operation which operates on all elements except the elements of the $m\xi$-column and $m\xi$-row. Further it is easy to prove that

$$\delta_{m\xi}|\text{all}| = -2\mathbf{k}_m\delta\boldsymbol{\tau}\,|m\eta;\ m\eta| + \delta_{m\xi;m\eta}|\text{all}|\,.$$

* If $|m\xi';\ 0\xi|^{(\alpha)} = 0$, $D_{m\xi'}/D_{0\xi}$ cannot be derived uniquely. In this case, $D_{m\xi'}$ is considered to be independent of $D_{0\xi}$ and to be given by the boundary conditions.

† If we take $\sum_{m\xi}|D_{m\xi}|^2 = 1$, the constant in equation (11) is $1/\sum_{m\xi}|m\xi;\ m\xi|$.

Thus we obtain finally

$$\delta|\text{all}| = -2 \sum_{m\xi} \mathbf{k}_m |m\xi;\, m\xi| \delta\boldsymbol{\tau} = 0 \tag{13'}$$

as the equation of the tangential plane of the dispersion surface.

4. Conclusion and discussion

Comparing (12) and (13′), we can conclude that

$$(\boldsymbol{\gamma} \cdot \delta\boldsymbol{\tau}) = 0\,. \tag{14}$$

This means that the direction of energy flow corresponding to each branch of the dispersion surface is normal to the tangential plane of the dispersion surface, in the case of a non-absorbing crystal.

The above conclusion may be understood also from the stand-point of wave packets. In the previous work on electron diffraction, the author pointed out (1952) that electron wave packets go through a crystal in the direction of the normal of the dispersion surface. This holds also in the case of X-ray diffraction. Therefore equation (14) may be considered as another proof of the previous result.

It seems worth while to note here that a similar situation of energy flow in crystal takes place also in the case of visible rays. As is well known (Szivessy, 1929), the normal surface (Normalenfläche), ray surface (Strahlenfläche) and index surface (Indexfläche) are considered to describe the geometrical relations of propagation of waves and rays. In the usual texts on crystal optics, it is shown that waves propagate so that their wave-vectors $\mathbf{K}$ lie in the direction of the normal of the ray surface. This is proved (Born, 1933) from the following fundamental relation of the field vector in crystals

$$c^2\mathbf{E} = (\mathbf{r} \times (\mathbf{D} \times \mathbf{r}))\,, \tag{15}$$

where $\mathbf{E}$ is the electric vector, c is the light velocity in vacuum and $\mathbf{r}$ is the radius vector of the ray surface. By a quite similar procedure we can prove the corresponding relations that rays propagate in the direction of the normal of the dispersion surface from the following relation

$$(\omega/c)^2\mathbf{D} = (\mathbf{k} \times (\mathbf{E} \times \mathbf{k}))\,, \tag{16}$$

where ω is angular frequency and $\mathbf{k}$ is the radius vector of the dispersion surface. In crystal optics of visible rays the index surface is used instead of the dispersion surface but they are geometrically similar to each other.

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