Acta Cryst. (1958). **11**, 888

Group Velocity and Phase Velocity in X-ray Crystal Optics

BY P. P. EWALD

Polytechnic Institute of Brooklyn, 333 Jay Street, Brooklyn 1, N.Y., U.S.A.

(*Received* 1 *February* 1958)

In a Laue type diffraction experiment in which a secondary ray is split from the primary one the propagation of energy takes place along the net planes on which reflection occurs, rather than along the normals of the incident or reflected waves. It is shown that this result follows directly from the existence of a surface of dispersion if bundles of waves of small angular opening $d\Omega$ are substituted for the strictly plane component waves of the X-optical field. The direction of the group velocity is defined for each bundle and is shown to be directed along the normal to the Surface of Dispersion (or Index Surface in Light Optics) at the point of this surface which represents one of the component plane-wave fields. The same result has been achieved by M. v. Laue in a discussion of G. Borrmann's experiments, and, recently, by N. Kato for electron and X-ray diffraction. The present treatment, based on the concept of group-velocity, is more general and requires no detailed calculation of the field.

A further result of N. Kato, regarding the propagation of a field of finite width, as cut out by a slit, is also given an interpretation by inspection.

Introduction

N. Kato (1958) has pointed out in the preceding paper that the surface in Fourier space which is usually called the Surface of Dispersion in the dynamical theory of X-rays fulfills the same function as the Index Surface in ordinary crystal optics. Any point A of the surface of dispersion is the origin of wave vectors $\mathbf{K}_h$ leading from A to various points $\mathbf{h}$ $(= (h_1h_2h_3))$ of the reciprocal lattice, whereby the origin O is always included. For monochromatic X-rays all the magnitudes $|\mathbf{K}_h|$ are very nearly $k_0 = \nu/c$, the wave constant for a wave of frequency ν travelling through empty space, and this condition limits the number of co-existent wave vectors. The difference between $|\mathbf{K}_h|$ and k_o gives rise to the refractive index $\mu_h = |\mathbf{K}_h|/k_0$ of each wave and also determines the relative amplitudes of the waves represented by the point A. These plane monochromatic waves form the simplest dynamically consistent X-optical field in an unbounded crystal. In the light-optical case k_0 is so small that only the vector from a point A of the surface of dispersion to the origin O of Fourier space (and of the reciprocal lattice) comes close enough to length k_0 and the optical field therefore consists of a single wave instead of, say, n in the X-ray case. While in the latter case the surface of dispersion has $2n$ sheets, there are only two sheets in the case of light. A line drawn into O has two intersections with the surface in the case of light and gives rise to two vectors $\mathbf{K}$, $\mathbf{K}'$ of different lengths and to two values of the refractive index for waves having the direction of the line as wave-normal. For this reason the two-sheet surface is called the Index Surface. Its main use in crystal optics is for the construction of the refracted rays, given the direction of incidence on a plane surface. This is a direct generalization of Snell's construction giving the same result for an isotropic medium.

N. Kato (1952) has studied for electron diffraction what happens to an incident wave which is cut out from an unbounded wavefront by a slit or other form of diaphragm. He has hereby reached the conclusion that in the case of a field consisting of two coupled plane waves the stream of particles or the energy travels in a direction which differs from those of the two wave vectors and is that of the normal to the surface of dispersion. This result is closely related to the demonstration by Borrmann (1950) that in the case of the Borrmann effect the rays emerge from the underside of a crystal as if they had traversed its thickness along the reflecting net planes. M.v.Laue (1952) was the first to explain this on the basis of the dynamical theory including absorption, and others arrived at the same conclusion, including Kato.

All these papers are based on rather detailed and complicated calculations. But the basic fact, leading to their main result, can be obtained in a very simple way—and this is the justification of this note. It is merely a matter of distinguishing between group velocity and phase velocity.

Two methods of studying the propagation of rays (energy)

The propagation of energy in an optical field may be obtained by two different procedures which can be shown generally to lead to the same result.

(i) The first, which has been followed in the papers referred to above, is to calculate Poynting's vector of energy flux. Even in the simple case of considering a field consisting of only two plane-wave components

the Poynting vector is quite complicated. It has been plotted a long time ago by Eichenwald (1912) and these diagrams are not only very instructive for the case of the reflection of light from a plane surface, for which they were drawn, but they are also applicable to the case of X-ray reflection with only slight modifications. The instantaneous picture of the tubes of energy flow is entirely different from what would be naïvely expected to indicate energy incident in one direction and reflected in another. Such a simple result can only be obtained by a radical process of space- and time-averaging which obliterates most of the details presented in the instantaneous diagram. It is precisely such averaging that is applied in the above papers. The discussion of a monochromatic optical field consisting of plane waves is sufficient for obtaining the results.

(ii) The second procedure for discussing the propagation of energy in an optical field is that of considering the displacement of a wave-packet. This was first done by Lord Rayleigh for strictly plane waves which are not monochromatic. Such waves are represented by a Fourier integral in frequency space, such as

$$u(x,t) = \int A(\nu) \exp\left[-j(\nu t - kx)\right] d\nu, \quad (j = 2\pi i). \qquad (1)$$

If $A(\nu)$ is large only within a small frequency range the phases of the component waves, which are contained in the complex amplitudes $A(\nu)$, may, at a certain time t_0 and place x_0 be largely compensated or complemented by the exponential, so that an especially large value of $u(x_0, t_0)$ results. We can follow the course of this large value—ignoring an uninteresting phase factor—by making the change of phase of the integrand the same throughout the interval of integration when changing t_0, x_0 by $\Delta t, \Delta x$:

$$(d/d\nu)(\nu\Delta t - k\Delta x) = 0 \quad \text{or} \quad \Delta x/\Delta t = d\nu/dk\,. \qquad (2)$$

Clearly the energy which is contained in this large field value will propagate with the velocity prescribed by this condition, namely with phase velocity $q = \nu/k$ if the relation between ν and k is linear (no dispersion), and with group velocity $g = d\nu/dk$ in the case of a non-linear relation (dispersion).

In a dispersive medium the wave-packet represented by (1) travels, like all its component waves, in the x-direction, but stays together only for a limited length and time because of the approximative character of the condition (2).

Substitution of wave bundles for plane waves

The usual method of considering monochromatic plane waves as the elementary form of field in optics leads to difficulties as soon as energy considerations are the primary aim. This is well known in the theory of Black Body Radiation where the elements considered are bundles of plane waves of angular opening $d\Omega$ and of frequency interval $d\nu$. For the discussion of the propagation of fields, where linear superposition holds, the plane monochromatic wave is convenient and implies no restriction, since the energetically move significant fields can be built up from plane monochromatic waves by Fourier's theorem. Where the speed of energy transport is important—as in discussing the measurements of the velocity of light—the use of a frequency interval is imperative, because only in that way can a recognizable wave-packet or signal be built up. On the other hand the discussion of the geometrical path of energy in X-ray, or of charge in electron diffraction only requires the consideration of an elementary field having an angular opening. Polychromatism would need to be introduced only if the velocity of propagation were actually measured. This has so far not been attempted, though it seems feasible for electron and neutron diffraction by the use of a chopper.

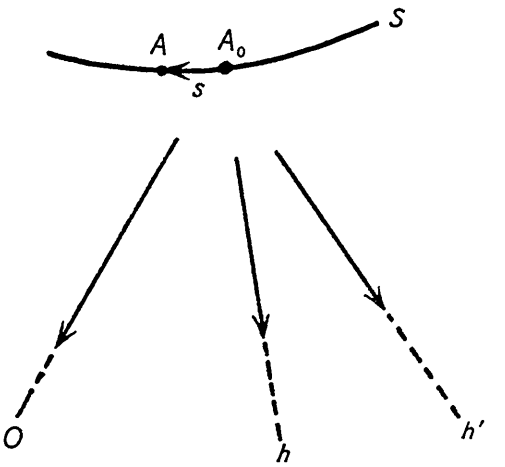

Fig. 1. Part of the surface of dispersion S with points A_0 and A, each representing an optical field consisting of plane waves with wave-vectors ending in the (distant) lattice points O, h, h' in Fourier space.

Let S in Fig. 1 be part of the surface of dispersion for X-rays and let the vectors

$$\overrightarrow{A_0O} = \mathbf{K}_1, \quad \overrightarrow{A_0h} = \mathbf{K}_h, \quad \overrightarrow{A_0h'} = \mathbf{K}_{h'}, \ldots$$

be the wave vectors of the plane monochromatic waves forming an elementary field in the dynamical theory. To the scale used for S, these vectors would have to be about a mile long. The field, including the relative amplitudes and phases of the plane waves is fully represented by the point A_0 and the position of A_0 on S guarantees the dynamical consistency of the field.

Next shift A_0 to A by a vector $\mathbf{s}$, lying in S. A again represents a consistent field, whose wave vectors are $(-\mathbf{s}+\mathbf{K}_1)$, $(-\mathbf{s}+\mathbf{K}_h)$, ... etc. The amplitude ratios of the plane waves of this field differ from those of the previous one, and each field can, of course, be given an arbitrary overall amplitude and phase.

By varying the position of A throughout a small

area of S, each of the original plane waves of the field A_0 will be replaced by a bundle of plane waves with wave-vectors varying within certain solid angles. The field in—approximately—the direction $\mathbf{K}_h$ is then described by

$$u_h(\mathbf{x}, t) = \int B_h(\mathbf{s}) \exp\left[-j(\nu t - (\mathbf{K}_h - \mathbf{s}) \cdot \mathbf{x})\right] d^2s \,,$$

where $B_h(\mathbf{s})$ is the amplitude of the wave associated with the direction $\mathbf{K}_h$ and the shift $\mathbf{s}$. d^2s is the element of area of S. The entire optical field is obtained by summation over h $(= 0, h, h', \ldots)$.

The above expression can be interpreted as a wave travelling in the direction of $\mathbf{K}_h$ and having a slowly varying amplitude:

$$u_h(\mathbf{x}, t) = \exp\left[-j(\nu t - \mathbf{K}_h \cdot \mathbf{x})\right] \int B_h(\mathbf{s}) \exp\left[-j\mathbf{s} \cdot \mathbf{x}\right] d^2s \,.$$

The dependence of the amplitude integral on $\mathbf{x}$ contains the local fluctuations of the field strength. The places where the field builds up to a large value depend on the amplitude and phase distribution assumed for the various points A. Irrespective of this we see, however, that in order to retain the same value of the amplitude we have to shift $\mathbf{x}$ so that the scalar product $\mathbf{s} \cdot \mathbf{x}$ is not changed. Since $\mathbf{s}$ lies in the surface of dispersion, $\mathbf{x}$ has to be shifted parallel to the normal of the surface of dispersion at the point A_0. Any signal we implant on the wave-front therefore travels in the direction of this normal.

It will be seen that this holds for each one of the directions $\mathbf{K}_h$. The place $\mathbf{x}$ where e.g. a field larger than average is built up, will vary from one bundle of waves to the other, since it depends on the B_h values. But for all waves the direction of energy flow is along the same normal to the surface of dispersion. Owing to the curvature of the surface of dispersion a signal will gradually change as it progresses. Its range is the shorter the greater the curvature of the surface of dispersion is at the central point A_0 of Fig. 1.

The same arguments can be applied to the Index Surface in the light-optical case: the ray direction associated with a direction of the wave-normal is found as the normal of the tangent plane of the index surface at the point where it is intersected by the wave-normal.

Applications

1) In the case of a simple Bragg reflection of order h of a plane-polarized ray the surface of dispersion has the well known shape of a hyperbolic cylinder shown in cross section in Fig. 2. The asymptotic lines are normal to the directions $\vec{AO}$ and $\vec{Ah}$. The normal to the surface of dispersion thus always lies between these directions. If $\mathbf{n}$ indicates the normal of a plane parallel crystal plate the relation between the fields outside and inside the crystal requires the use of two elementary consistent fields, represented by points A and A' on the two branches of the hyperbola so that

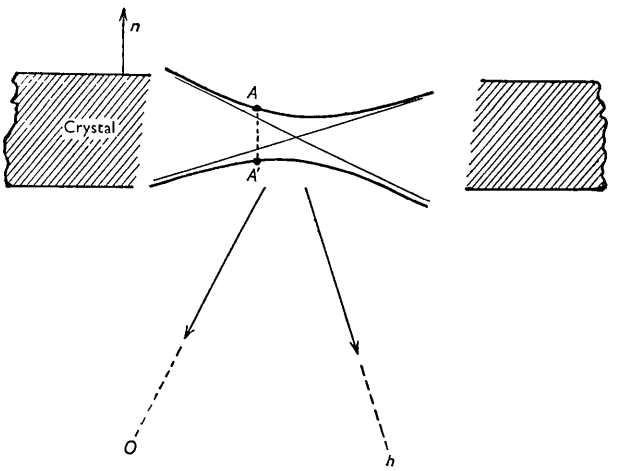

Fig. 2. Surface of dispersion for the case of one diffracted ray, shown simultaneously with the normal direction n of a crystal slab.

$A'A$ is parallel to $\mathbf{n}$. The direction of energy flux of field A shown in the figure lies close to the direction of the primary beam $\vec{AO}$, that of field A' close to $\vec{Ah}$, the direction of the diffracted beam. The position shown is towards one end of the range of reflection and the diffracted beam is weak; energy moves nearly in the direction of the primary beam. If the pair of points A, A' is shifted to the right, (corresponding to an increase of the glancing angle of the incident beam on the reflecting net planes), interaction between primary and diffracted beam increases and when A, A' lie near the vertices of the hyperbola the direction of energy flow is in both fields nearly along the reflecting planes (strictly so in the case of symmetrical reflection).

2) A beautiful result of N. Kato's (1952) study of the field generated by an incident wave of finite lateral extension (limitation by slit) shows that large values of the field within the crystal occur only in that region of the crystal which can be reached from the entrance port by progressing along the direction normal to the surface of dispersion. Fig. 3 shows this for symmetrical reflection. This result is understandable not only in terms of energy propagation, but also in terms of fields. For as soon as one of the wave-fronts gets out of the central region (vertically shaded), it is without its coupled companion wave; it is therefore reflected unbalanced into the other direction. Thus every element of wave-front exceeding the central region swerves round to head for it again. The interaction between the waves is thus prolonged against what it would seem according to a crude geometrical construction shown in Fig. 3 by the doubly shaded region. This discovery resolves the riddle why it is permissible to apply the formulae of the dynamical theory when using a narrow slit and a thick crystal, for instance in calculating the Borrmann effect, or in spectroscopy.

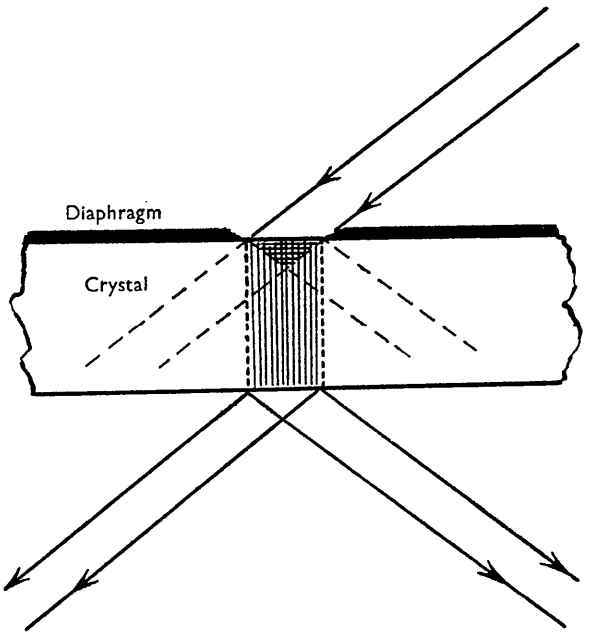

Fig. 3. Incidence of a ray limited sidewise and giving rise to symmetric reflection. The region of interaction is shaded vertically.

3) *Borrmann effect.* In the case of a crystal with absorbing atoms the optical fields represented by the points A and A' of Fig. 2 are differently affected by absorption. To understand this we recall that the formation of the field amplitude of each of the constituent plane waves is regulated by a 'resonance factor' $(\mathbf{K}_h^2-k_0^2)^{-1}$, where $\mathbf{K}_h$ is the wave-vector of the wave (and of the corresponding dipole phase of the atomic scatterers), and k_0 is the wave constant for propagation in empty space. If the 'Laue-point' is defined as the point in the plane of Fig. 2 which has exactly the distance k_0 from O and from h, then one branch of the hyperbola will pass closer to the Laue point than the other. In the simple case of a lattice of non absorbing point atoms, and plane-polarized X-rays, one branch of the hyperbola passes through the Laue-point. For the other polarization, or when there is a structure factor $\neq 1$ this branch only approaches it closely. If the resonance factor is very large, even a very small dipole amplitude gives rise to a very large field amplitude. Or: the field amplitude required to balance the amplitude of an incident wave is obtained with less dipole amplitude the nearer the point A (or A') of Fig. 2 lies to the Laue-point. In the limit of A coinciding with the Laue-point no dipole amplitude at all is required to obtain a finite field. The crystal in that case is optically empty; both waves have wave vectors of length k_0 and travel with phase velocity c. An equivalent statement is in this case that each dipole lies at a node of the wavefield of electric vectors. For were it not so, the ensuing vibration of the dipoles would create an infinitely strong wave.

If we admit dissipation of energy by the dipoles, this is proportional to their amplitude. On that part of the hyperbola which passes close to the Laue-point the efficiency of the dipoles for field production is great, and their amplitude remains small; there is thus only little energy dissipation, and this branch of the hyperbola leads to fields with only slight absorption. In (hypothetical) cases when the representative point A coincides with the Laue-point itself, absorption in the crystal is zero, no matter how strong it may be for the individual dipole or atom.

In passing through a thick crystal slab only the field with the smallest absorption will survive. Therefore in the Borrmann experiment only the fields represented by a small region on that branch of the surface of dispersion which is nearest to the Laue-point are observed. The direction of energy flow for these fields is clearly very nearly along the reflecting net planes.

4) *Other types of waves.* The relation between wave-normal and ray has been shown to have a purely kinematical origin. The direction of the ray is always along the normal of the wave-vector surface. This holds in particular for long acoustic and for ultrasonic waves in crystals and should be observable in the latter case.

The author sincerely thanks Dr N. Kato for stimulating discussions.

References

BORRMANN, G. (1950). *Z. Phys.* **127**, 297.
EICHENWALD, A. (1912). *Festschrift Heinrich Weber gewidmet*, p. 37–56. Leipzig and Berlin: Teubner.
KATO, N. (1952). *J. Phys. Soc. Japan*, **7**, 397.
KATO, N. (1958). *Acta Cryst.* **11**, 885.
LAUE, M. v. (1952). *Acta Cryst.* **5**, 619.