Watanabe (1966). The curvature of the broad Kikuchi lines shown in Fig. 4 can therefore be interpreted as the overlap of the broadened fine structures seen in Fig. 3. The interpretation is qualitative, however, and any quantitative analyses of the diffraction patterns must await further theoretical understanding of the dynamic diffuse scattering of electrons.

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The Darwin Dynamical Theory of X-ray Diffraction*

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A simple alternative to the Ewald–von Laue dynamical theory of X-ray diffraction is described. Several of the more important features of dynamical diffraction, including anomalous transmission, diffraction in asymmetric Laue geometry, and the properties of the dispersion surface, are derived. The method involves the solution of a system of difference equations similar to those first solved by Darwin. The formalism of electromagnetic theory is avoided, and the result is achieved with no loss in rigor. In addition to its greater simplicity, the theory seems to be easier to modify to account for small deviations from perfect periodicity, which are difficult to account for in terms of the Ewald–von Laue treatment.

Introduction

The central problem of X-ray crystallography has traditionally been, given a specific array of centers of scattering factor f, to combine the amplitudes and phases of the resultant scattered waves in order to recover the diffraction pattern associated with the array. Neither quantum mechanics nor electromagnetic theory is normally invoked. The crystallographer simply takes f to be the ratio of the wave scattered by an atom to that scattered by a classical electron, and leaves its computation to the theoretical physicist. All of the electromagnetic and quantum theory of the problem is contained in the calculation of f.

The Ewald (1916)–von Laue (1931) dynamical diffraction theory is a departure from this custom. Here, in order to obtain the total wave field inside a perfect crystal, one solves Maxwell's equations in a medium with a periodic, time dependent, complex dielectric constant. The treatment is elegant but rather involved.

We here show that that is not necessary, that all of the features of dynamical diffraction including the anomalous aspects of the Borrmann effect are recoverable with the usual tools of X-ray crystallography. No electromagnetic theory is used. The result is achieved by simply solving in Laue geometry the difference equations first solved by Darwin (1914) in Bragg geometry.

It has previously been shown (Borie, 1966) that at the precise Bragg angle for the symmetrical Laue case, such a procedure leads to the vanishing of the linear absorption coefficient and the anomalous behavior of the refractive index associated with the Borrmann effect. In this paper we compute the wave field for an arbitrary direction of incidence. Diffraction in asymmetric Laue geometry is discussed. We examine the behavior of the wave field in the immediate vicinity of the Bragg reflection for the symmetrical Laue case, and we derive the properties of the dispersion surfaces. The result is identical with that of the Ewald–von Laue theory.

Fresnel diffraction in transmission

A preliminary to writing the Darwin difference equations is to calculate the wave scattered by a single plane of scattering material. A family of such planes is then assembled to form a crystal, and the combination of the amplitudes and phases of the scattered waves is expressed by the difference equations.

This is conventionally done in reflection, or Bragg geometry (James, 1950), as illustrated in Fig. 1. The xy plane is populated by a uniform distribution of

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classical electrons, n per unit area, and is irradiated by a point source at S. We compute the scattered wave at P. The rays $SO=R$ and $OP=r$, in the xz plane and making equal angles θ_1 with the z axis, define the shortest path length from S to P *via* the plane. For a path length *via* the point (x,y) it is easy to show that

$$R_{xy}=R+x\sin\theta_1+\frac{x^2\cos^2\theta_1+y^2}{2R}$$

and

$$r_{xy}=r-x\sin\theta_1+\frac{x^2\cos^2\theta_1+y^2}{2r}.$$

In the above expressions x and y are assumed to be small compared with R and r so that terms beyond those quadratic in x or y may be neglected. The increase in path length, $\gamma=R_{xy}+r_{xy}-R-r$, after R is allowed to approach infinity so that the incident wave is plane, is then simply given by

$$\gamma(x,y)=\frac{x^2\cos^2\theta_1+y^2}{2r}.$$

The electron plane may then be divided into Fresnel zones. The first zone is contained within the ellipse whose equation is

$$\frac{\lambda}{2}=\frac{x^2\cos^2\theta_1+y^2}{2r}.$$

Standard Fresnel zone construction and Thomson scattering theory then give

$$A=A_0\frac{in\lambda\mathscr{K}}{\cos\theta_1}\frac{e^2}{mc^2}\exp\left[-\frac{2\pi i}{\lambda}r\right].$$

A is the net electric field at r, aside from a time factor, and A_0 is that of the incident plane wave just above the electron plane. $\mathscr{K}$ is a polarization factor, and is 1 or $\cos(\pi-2\theta_1)$ depending on whether the electric vector of the incident wave is parallel to the y axis of Fig. 1, or in the xz plane. If we replace each electron by an atom of scattering factor $f(\pi-2\theta_1)$, we obtain for the ratio of the amplitude of the scattered plane wave just above the plane to that of the incident wave just before its encounter with the plane

$$\frac{A}{A_0}=iq=i\frac{n\lambda\mathscr{K}}{\cos\theta_1}\frac{e^2f(\pi-2\theta_1)}{mc^2}.$$

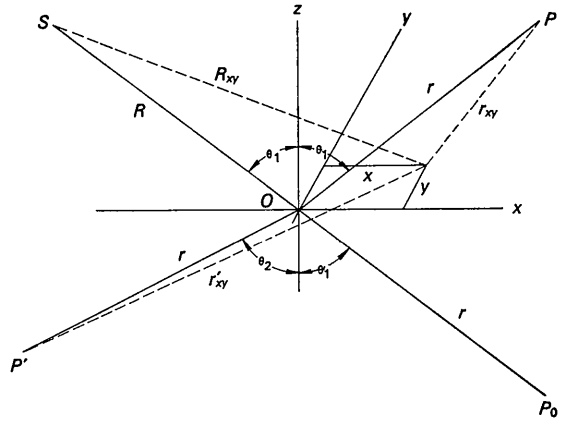

Fig. 1. Schematic illustration of Fresnel diffraction from a single plane of scattering centers.

iq is the complex single plane reflection coefficient. The factor i accounts for a phase advance of $\pi/2$ in the reflected wave relative to the incident wave.

The problem of computing the scattered wave at P_0, in the direction of the incident radiation, is parallel to the above discussed calculation. The resultant single plane coefficient in that case is

$$ig_0=i\frac{n\lambda}{\cos\theta_1}\frac{e^2f(0)}{mc^2}. \tag{1}$$

The above results are independent of the way the atoms are distributed in the plane. The only requirement is that any structure in the distribution be on a scale small compared with the dimensions of the Fresnel zone, which for X-rays are of the order of 10^{-4} cm.

We now ask whether by distributing the atoms in the plane in a special way, we can cause still a third scattered wave to occur. In particular we ask whether we can cause a plane wave in the direction OP', as shown in Fig. 1. OP' lies in the xz plane and makes an angle θ_2, as yet unspecified, with the z axis. For simplicity we take the three points P_0, P, and P' to lie the same distance r from O. Then

$$r'_{xy}=r+x\sin\theta_2+\frac{x^2\cos^2\theta_2+y^2}{2r}$$

and

$$\gamma(x,y)=\frac{x^2\cos^2\theta_2+y^2}{2r}+x(\sin\theta_1+\sin\theta_2).$$

This means that as x increases, the path length to P' increases very much more rapidly than to P or P_0.

Now suppose that we distribute the scattering centers in the xy plane only along lines parallel to the y axis, equally spaced, a_1 apart. Then the only relevant values of x are $x=ma_1$, where m is an integer. And suppose that we choose θ_2 so that

$$a_1(\sin\theta_1+\sin\theta_2)=h\lambda \tag{2}$$

where h is an integer. Then

$$\gamma(x,y)=\frac{x^2\cos^2\theta_2+y^2}{2r}+hm\lambda.$$

This is identical with the path length change to P except that θ_1 is replaced with θ_2, and an integral number of wavelengths are added on. Hence the phases combine at P' exactly as they do at P. The rest of the derivation goes exactly as before. We may construct an elliptical pseudo-Fresnel zone for the direction OP'. It is a pseudo-zone because as we move from O out to the edge of the zone the path length increase may be very much greater than $\lambda/2$. But we have situated the scattering centers so that the path length change is exactly the same as it would be for reflection at angle θ_2, plus exactly an integral number of wave-

lengths. The resultant expression for the complex single plane transmission coefficient is

$$ig = i\frac{n\lambda\mathscr{K}}{\cos\theta_2}\frac{e^2 f(\theta_1+\theta_2)}{mc^2}. \quad (3)$$

Here the polarization factor $\mathscr{K}$ is either 1 or $\cos(\theta_1+\theta_2)$. Note that though we have confined the scattering centers to lines in the xy plane, we have not required that all the electron density be so confined. The atomic scattering factor f accounts for the spatial distribution of the electron cloud, and with its use we may treat the atom as a point scatterer.

We may now combine a family of such planes to form a crystal, as shown in Fig. 2, and ask what the conditions are for constructive interference in the directions θ_1 and θ_2. If the planes are spaced properly, reinforcement occurs in the θ_1 direction, and the standard Darwin treatment for Bragg geometry results. We are here interested only in the Laue case, that is, reinforcement in the θ_2 direction. In what follows we shall assume that the scattered waves q always interfere destructively, and we shall ignore them.

The difference equations and their solution

The planes of Fig. 2 are numbered $0,1,2,\ldots,r,\ldots$ Let T_r be the displacement of the wave in the direction of the incident radiation, defined by θ_1, just before the rth plane. T_0 then is the displacement in free space just before the wave encounters the crystal. The phase retardation in T corresponding to a translation from the rth to the $(r+1)$th plane is

$$\varphi_1 = \frac{2\pi a_2}{\lambda}\cos\theta_1. \quad (4)$$

It has been shown that scattered plane waves, in a direction θ_2 related to θ_1 by equation (2), will result from the interaction of the wave T with the planes. Let S_r be the displacement for the resultant wave in the θ_2 direction just after the rth plane. The phase retardation in S for a translation between planes is

$$\varphi_2 = \frac{2\pi a_2}{\lambda}\cos\theta_2. \quad (5)$$

S_r is composed of that part of T_r which is scattered in the θ_2 direction by the rth plane, plus that part of S_{r-1} which is transmitted by the rth plane. Hence

$$S_r = igT_r + S_{r-1}(1+ig_0)\exp(-i\varphi_2). \quad (6)$$

T_{r+1} is that part of T_r which is transmitted by the rth plane plus that part of S_{r-1} which is scattered in the θ_1 direction by the rth plane:

$$T_{r+1} = T_r(1+ig_0)\exp(-i\varphi_1) + igS_{r-1}\exp[-i(\varphi_1+\varphi_2)]. \quad (7)$$

Equations (6) and (7) may be combined to obtain an equation in T only:

$$T_{r+2} = T_r\exp[-i(\varphi_1+\varphi_2)][(ig)^2-(1+ig_0)^2] + T_{r+1}(1+ig_0)[\exp(-i\varphi_1)+\exp(-i\varphi_2)]. \quad (8)$$

The general solution to a difference equation of this form is $T_r = C\beta^r$ where C and β are constants. Its substitution into equation (8) yields

$$\beta^2 - \beta[2(1+ig_0)\exp(-i\varphi_0)\cos\Delta\varphi] - \exp(-2i\varphi_0)[(ig)^2-(1+ig_0)^2] = 0.$$

In the above, $\varphi_0 = \frac{1}{2}(\varphi_1+\varphi_2)$ and $\Delta\varphi = \frac{1}{2}(\varphi_1-\varphi_2)$. The solution to the quadratic equation in β is

$$\beta = \exp(-i\varphi_0)\{(1+ig_0)\cos\Delta\varphi \pm i[g^2+(1+ig_0)^2\sin^2\Delta\varphi]^{\frac{1}{2}}\}. \quad (9)$$

With β_1 corresponding to the positive choice of sign in (9), we have that $T_r = C_1\beta_1^r + C_2\beta_2^r$. With the boundary conditions that $T_0 = 1$ and $S_{-1} = 0$, there results

$$C_1 = \tfrac{1}{2}\left\{1 - \frac{(1+ig_0)\sin\Delta\varphi}{[g^2+(1+ig_0)^2\sin^2\Delta\varphi]^{\frac{1}{2}}}\right\}$$

and

$$C_2 = \tfrac{1}{2}\left\{1 + \frac{(1+ig_0)\sin\Delta\varphi}{[g^2+(1+ig_0)^2\sin^2\Delta\varphi]^{\frac{1}{2}}}\right\}.$$

If the solution for T_r is substituted into equation (7), we obtain an expression for S. After some simplification there results

$$T_r = \tfrac{1}{2}\left\{1 - \frac{(1+ig_0)\sin\Delta\varphi}{[g^2+(1+ig_0)^2\sin^2\Delta\varphi]^{\frac{1}{2}}}\right\}\beta_1^r + \tfrac{1}{2}\left\{1 + \frac{(1+ig_0)\sin\Delta\varphi}{[g^2+(1+ig_0)^2\sin^2\Delta\varphi]^{\frac{1}{2}}}\right\}\beta_2^r \quad (10)$$

and

$$S_{r-1}\exp(-i\varphi_0) = \tfrac{1}{2}\frac{g}{[g^2+(1+ig_0)^2\sin^2\Delta\varphi]^{\frac{1}{2}}}\beta_1^r - \tfrac{1}{2}\frac{g}{[g^2+(1+ig_0)^2\sin^2\Delta\varphi]^{\frac{1}{2}}}\beta_2^r. \quad (11)$$

Internal diffraction in asymmetric Laue geometry

It is apparent from equations (10) and (11) that there is a significant wave in the S direction at $\Delta\varphi = 0$. This situation corresponds to $\theta_1 = \theta_2$ and equation (2) simply reduces to Bragg's law for the $(h00)$ planes, which from Fig. 2 are normal to the crystal surface. However, it is

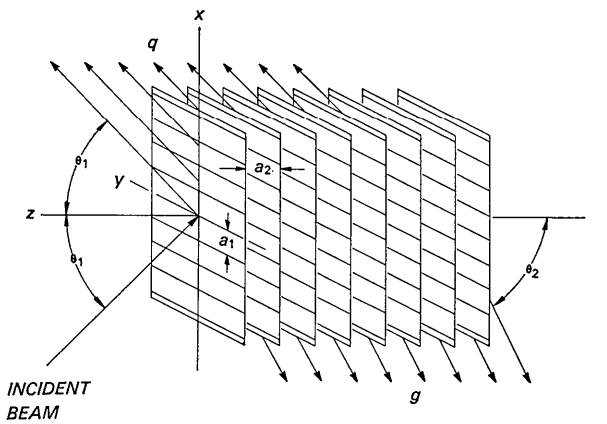

Fig. 2. Illustration of the combination of Fresnel diffracting planes to form a crystal.

also clear from (10) and (11) that S_r is 'turned on' not only near $\Delta\varphi=0$, but as well at $\Delta\varphi=k\pi$ where k is an integer. We show that this corresponds to diffraction from $(h\bar{k}0)$ planes, that is, diffraction in asymmetric Laue geometry.

If we let unit vectors $\mathbf{s}$ and $\mathbf{s}_0$ define the directions of the S and T waves so that $\mathbf{s}\,.\,\mathbf{a}_1=a_1\sin\theta_2$ and $\mathbf{s}_0\,.\,\mathbf{a}_1=-a_1\sin\theta_1$, equation (2) may be written

$$\mathbf{a}_1\,.\left(\frac{\mathbf{s}-\mathbf{s}_0}{\lambda}\right)=h\,. \tag{12}$$

From the definition of $\Delta\varphi$ we have that

$$\Delta\varphi=\tfrac{1}{2}(\varphi_1-\varphi_2)=k\pi\,,$$

which, with the aid of equations (4) and (5), may be written

$$\frac{a_2\cos\theta_2}{\lambda}-\frac{a_2\cos\theta_1}{\lambda}=-k\,.$$

In terms of $\mathbf{s}$ and $\mathbf{s}_0$ this becomes

$$\mathbf{a}_2\,.\,\frac{\mathbf{s}-\mathbf{s}_0}{\lambda}=-k\,. \tag{13}$$

Equations (12) and (13) describe the components of the diffraction vector parallel to $\mathbf{a}_1$ and $\mathbf{a}_2$. Hence in terms of the reciprocal vectors $\mathbf{b}_1$ and $\mathbf{b}_2$ it may be written

$$\frac{\mathbf{s}-\mathbf{s}_0}{\lambda}=h\mathbf{b}_1-k\mathbf{b}_2\,,$$

which is simply a statement of Bragg's law for the $(h\bar{k}0)$ planes.

The internal wave field in the the absence of diffraction

If $\Delta\varphi$ is not a multiple of π so that $\sin^2\Delta\varphi\gg g^2$, the coefficients of β_1^r and β_2^r in equation (11) are very small and the diffracted wave vanishes. The coefficient of β_1^r in equation (10) is also very small, while that of β_2^r is nearly unity. Hence (10) reduces to $T_r=\beta_2^r$ and equation (9) becomes

$$\beta_2=\exp(-i\varphi_0)\{(1+ig_0)\cos\Delta\varphi - i(1+ig_0)\sin\Delta\varphi\}=\exp(-i\varphi_1)\exp(ig_0) \tag{14}$$

since g_0 is sufficiently small that $1+ig_0$ may be written $\exp(ig_0)$.

Thus the phase retardation experienced by T_r as r is advanced to $r+1$ is not φ_1, as we would expect in free space, but φ_1-g_0. We may think of this as a small *advance* in phase g_0 of the wave front each time it passes through a plane of scattering material, as illustrated in Fig. 3. This causes the effective wave front, and hence the wave propagation vector, to be rotated through a small angle η_0, which gives rise to the normal refractive index n of the medium. From Snell's law

$$n=\sin\theta_1/\sin(\theta_1+\eta_0)\simeq 1-\eta_0\cot\theta_1$$

since η_0 is very small. If δ_0 is the defect from unity in n so that $\delta_0=1-n$, we have that

$$\delta_0=\eta_0\cot\theta_1\,. \tag{15}$$

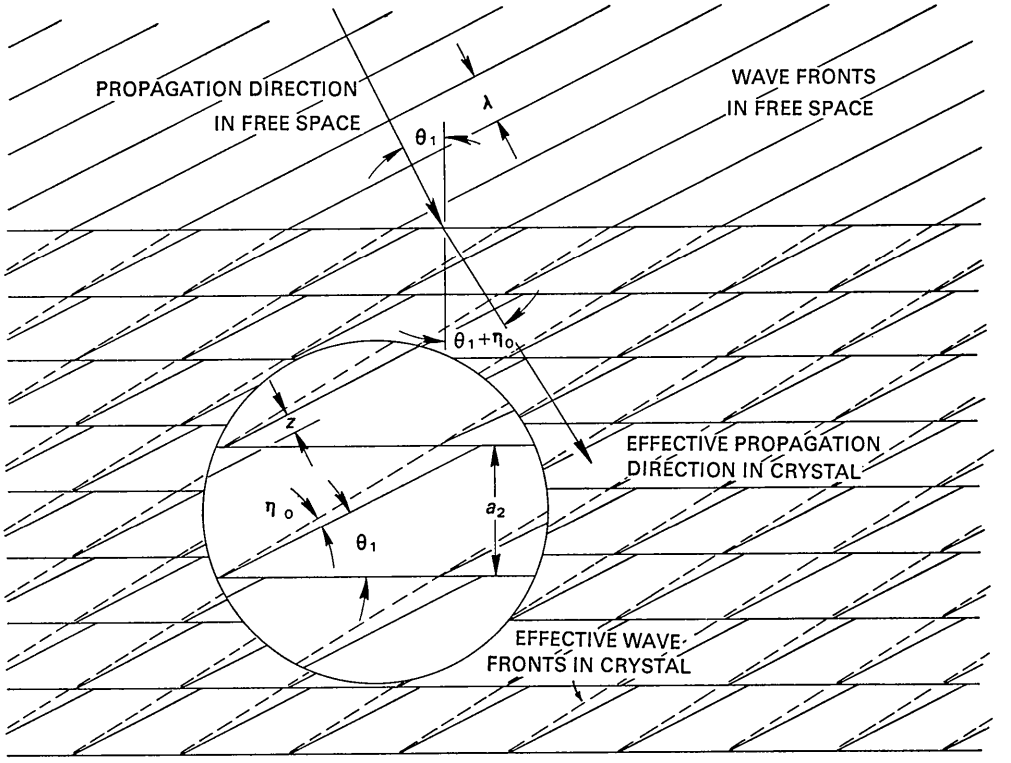

Fig. 3. Illustration of the relation between the phase advance on transmission through a scattering plane and the index of refraction.

If z (Fig. 3) is the actual linear distance associated with the phase advance g_0 we have that

$$\eta_0 = \frac{z}{a_2/\sin\theta_1}$$

or, since $2\pi z/\lambda = g_0$,

$$\eta_0 = \frac{\left(\frac{g_0\lambda}{2\pi}\right)}{\left(\frac{a_2}{\sin\theta_1}\right)} = \frac{g_0\lambda\sin\theta_1}{2\pi a_2}. \tag{16}$$

Equations (1) and (16) may be substituted into (15) to obtain the usual expression for the refractive index defect.

Near a Bragg reflection the phase advance may take on an anomalous value p, in which case (15) and (16) become

$$\delta = \eta\cot\theta_1 \tag{17}$$

and

$$\eta = \frac{p\lambda\sin\theta_1}{2\pi a_2}. \tag{18}$$

If g_0 (or p) includes a small positive imaginary component it is clear from (14) that upon transmission through a plane the wave not only experiences a phase advance but is slightly attenuated as well. This attenuation is a consequence of the anomalous dispersion correction to f and gives rise to the usual linear absorption coefficient. If near a Bragg reflection a value of p obtains which is real, then the absorption coefficient vanishes and anomalous transmission results.

The existence of a wave point

In this and subsequent sections we consider the behavior of the wave field in the immediate vicinity of $\Delta\varphi = 0$, that is, near the condition for symmetrical Laue diffraction.

In elementary theory, in which refractive indices are ignored, the usual Ewald construction is as shown in Fig. 4(*a*). A sphere of radius $k_B = 1/\lambda$ (the free space wavelength) is drawn about the Laue point L. The wave propagation vectors of the incident and diffracted waves at the Bragg angle θ_0 are then $\mathbf{k}_B = LO$ and $\mathbf{k}_b' = LH$. Their difference is the reciprocal lattice vector OH.

Fig. 4(*b*) is an illustration of the actual situation in the immediate neighborhood of the Laue point. The incident radiation may deviate from θ_0 by a small angle $\Delta\theta$ so that $\theta_1 = \theta_0 - \Delta\theta$. If that is so the propagation vector of the incident radiation is given by $\mathbf{k}$ rather than $\mathbf{k}_B$ as shown. The magnitudes of $\mathbf{k}$ and $\mathbf{k}_B$ are of course equal.

Inside the crystal, because there is a refractive index defect δ associated with the incident radiation, the magnitude of its propagation vector is no longer k but $K = k(1-\delta)$. The line AB is a segment of a circle drawn about O of radius K, so that the terminal of $\mathbf{K}$ must lie somewhere on it. It may safely be drawn as a straight line because $\delta \ll 1$. Because of the refractive index the vector $\mathbf{K}$ is rotated relative to $\mathbf{k}$ through an angle η. According to the relation (17), this places the terminal of $\mathbf{K}$ at W. The direction of $\mathbf{K}$ is thus defined by the angle $\theta_0 - \Delta\theta + \eta$.

The question to be explored in this section is, given the above description of $\mathbf{K}$, how should the propagation vector $\mathbf{K}'$ of the diffracted wave inside the crystal be drawn? We show that as a consequence of equations (10) and (11), it must be drawn from the same point W.

It is clear from the construction of Fig. 4(*b*) that if $\mathbf{K}'$ does terminate at W, it will have associated with it a refractive index defect δ' different from δ and a direction given by $\theta_0 + \Delta\theta + \eta'$. Of course, η' must be related to δ' by (17). From the geometry of Fig. 4(*b*), δ and δ' must be related by

$$k\delta = k\delta' + k\Delta\theta\sin 2\theta_0 . \tag{19}$$

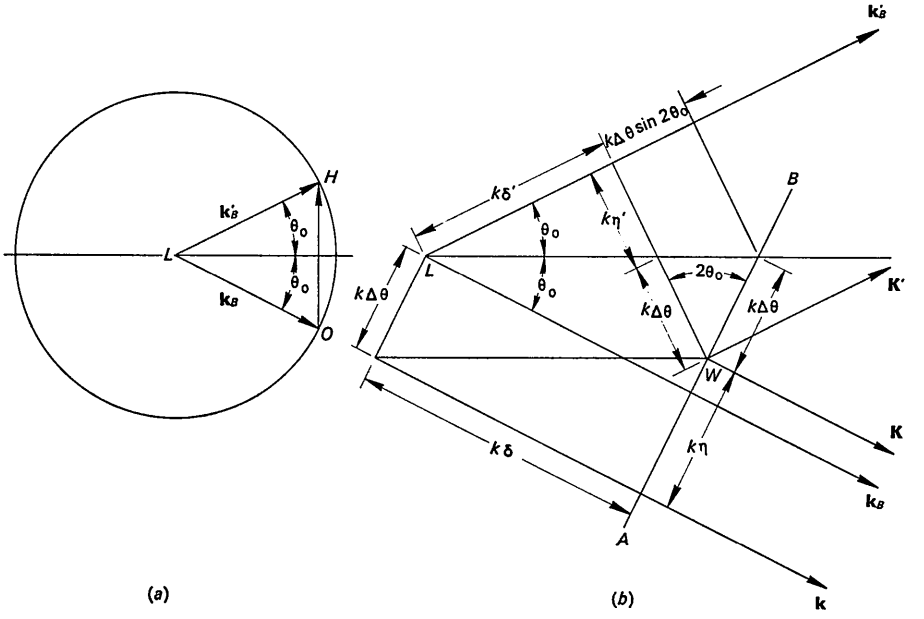

Fig. 4. (*a*) The Ewald sphere of reflection. (*b*) Construction illustrating the geometry in the neighborhood of the Laue point L and the wave point W.

We have seen that because of refraction, the phase retardation in T_r as r is advanced to $r+1$ is not φ_1 but $\Phi=\varphi_1-p=\varphi_0+\Delta\varphi-p$ where

$$\Delta\varphi=2\pi a_2 \sin\theta_0\Delta\theta/\lambda\,. \tag{20}$$

Similarly for S_r, $\Phi'=\varphi_0-\Delta\varphi-p'$.

But from equations (10) and (11), the same factors β_1 and β_2 describe both the T and S waves. Hence we must have that $\Phi=\Phi'$. This fact relates p and p', the phase advances experienced by T and S each time the wave fronts pass through a scattering plane:

$$p'=p-2\Delta\varphi\,.$$

With the aid of relations (17) and (18), p and p' may be expressed in terms of δ and δ', and $\Delta\varphi$ may be expressed in terms of $\Delta\theta$ with equation (20). The result is just equation (19), which we set out to prove. Thus $\mathbf{K}$ and $\mathbf{K}'$ must always terminate at a common point W, called the wave point, near the Laue point.

The dispersion equation

As the angle of incidence is varied in the vicinity of θ_0, the wave point moves in the neighborhood of the Laue point. We consider here the equation of its path.

We may think of T or S as the combination of two waves, each with a different refractive index. If we write $\beta_1=B_1\exp(-i\Phi_1)$ and $\beta_2=B_2\exp(-i\Phi_2)$, equation (10) becomes

$$T_r=C_1(B_1\exp(-i\Phi_1))^r+C_2(B_2\exp(-i\Phi_2))^r\,. \tag{22}$$

A similar expression for S_r may be written from equation (11) with different C's but the same values of β_1 and β_2. In equation (22), B_1 gives the attenuation per plane and Φ_1 the phase retardation per plane for one of the waves of which T_r is composed. The other component of T_r is similarly described by B_2 and Φ_2. Since the motion of the wave point in the vicinity of the Laue point depends on the behavior of the refractive index in that neighborhood, we are here concerned only with the values of the Φ's. Specifically we consider the behavior of Φ_2.

Because $\Delta\varphi$, g_0, and g are small quantities, for purposes of this discussion equation (9) may be written

$$\beta_2=\exp(-i\varphi_0)[1+ig_0-i(g^2+\Delta\varphi^2)^{\frac{1}{2}}]$$
$$\simeq\exp\{-i[\varphi_0-g_0+(g^2+\Delta\varphi^2)^{\frac{1}{2}}]\}\,.$$

Hence

$$\Phi_2=\varphi_0-g_0+[g^2+\Delta\varphi^2]^{\frac{1}{2}}\,. \tag{23}$$

If $\Delta\Phi$ is large compared with g, the value of the phase retardation per plane given by (23) reduces to $\varphi_0-g_0+\Delta\varphi=\varphi_1-g_0$, and the discussion leading to equations (15) and (16) follows. The refractive index defect for the β_2 component of T_r is a constant, δ_0, independent of the position of the wave point. Thus the wave point must move along the line VQ of Fig. 5. A similar consideration of β_1 shows that the wave point for that component of the wave field moves along the asymptote MQ.

The above described motion of the wave point breaks down in the neighborhood of the point Q, where $\Delta\varphi=0$. In that region we describe the position of the wave point in terms of the coordinates ξ_0 and ξ_H which give its perpendicular distance from the asymptotes VQ and MQ, as shown in Fig. 5. Here the phase retardation per plane must be written φ_1-p. This may be combined with equation (23) to give an expression for p:

$$p=g_0+\Delta\varphi-[\Delta\varphi^2+g^2]^{\frac{1}{2}}\,.$$

Equations (16) and (18) may be used to give

$$\eta=\eta_0-\Delta\eta \tag{24}$$

where

$$\Delta\eta=[(\Delta\varphi^2+g^2)^{\frac{1}{2}}-\Delta\varphi]\frac{\lambda\sin\theta_0}{2\pi a_2}\,. \tag{25}$$

From equations (15), (17), and (24) we have that

$$\delta=\delta_0-\Delta\eta\cot\theta_0\,.$$

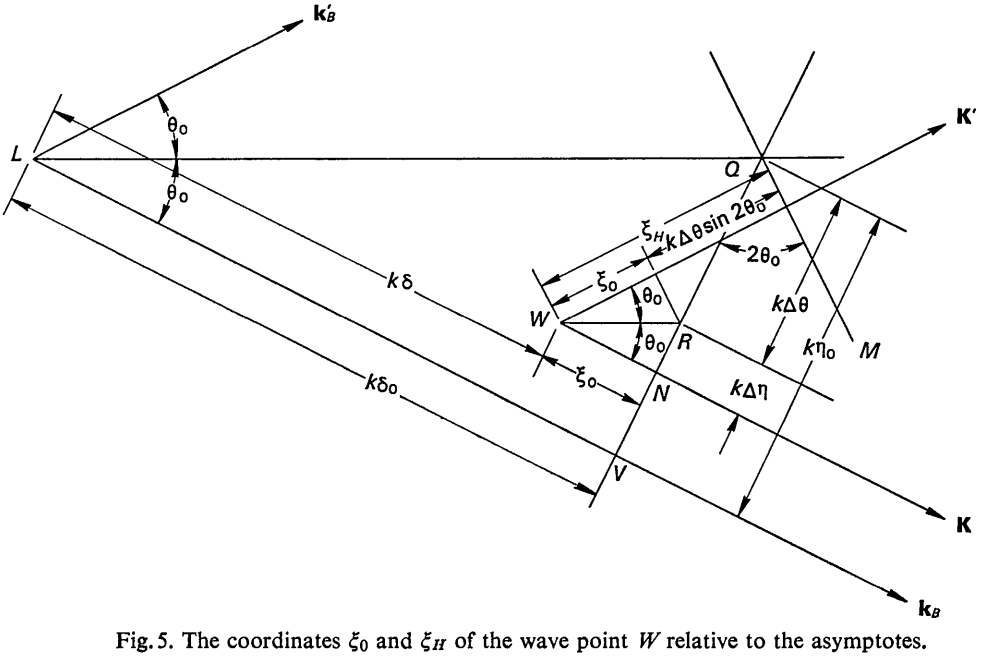

Fig. 5. The coordinates ξ_0 and ξ_H of the wave point W relative to the asymptotes.

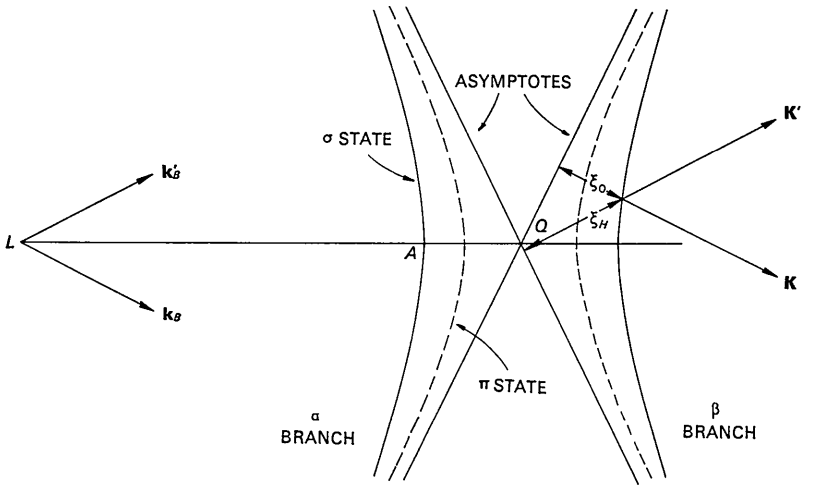

Fig. 6. The dispersion surfaces for both states of polarization.

Or, since from Fig. 5, $\xi_0=k(\delta_0-\delta)$,

$$\xi_0=k\Delta\eta\cot\theta_0\,. \tag{26}$$

Thus the distance NR must be $k\Delta\eta$ as shown. From equation (15), the distance $VQ=k\eta_0$, and if the wave point is at W, then RQ must be $k\Delta\theta$. From the geometry of the figure it follows that

$$\xi_H=\xi_0+k\Delta\theta\sin 2\theta_0=\xi_0+2k\Delta\theta\sin\theta_0\cos\theta_0\,. \tag{27}$$

Equation (25) may be used to eliminate $\Delta\eta$ from (26):

$$\xi_0+\frac{k\lambda\Delta\varphi\cos\theta_0}{2\pi a_2}=\frac{k\lambda\cos\theta_0(\Delta\varphi^2+g^2)^{\frac{1}{2}}}{2\pi a_2}\,.$$

After squaring both sides and eliminating $\Delta\varphi$ in terms of $\Delta\theta$ with equation (20), there results

$$\xi_0(\xi_0+2k\Delta\theta\sin\theta_0\cos\theta_0)=\frac{k^2\lambda^2\cos^2\theta_0 g^2}{4\pi^2a_2^2}\,.$$

From (27) the left side of the above equation may be written $\xi_0\xi_H$. If the value of g quoted in equation (3) is used, there results

$$\xi_0\xi_H=\frac{N^2\lambda^2f^2e^4\mathscr{K}^2}{4\pi^2m^2c^4}\,. \tag{28}$$

In the above, n/a_2, the number of atoms per unit volume, is written as N. This expression defines one branch of a hyperbola along which the wave point moves. Its other branch results from a consideration of β_1 parallel to the above. Equation (28) is identical with the result of the Ewald–von Laue theory (Batterman & Cole, 1964), and represents a section through the dispersion surface. This section is illustrated in Fig. 6. Because $\mathscr{K}$ may be either 1 (σ state of polarization) or $\cos 2\theta_0$ (π state) depending on the direction of the electric vector, for unpolarized incident radiation two hyperbolae must be drawn as shown. If the imaginary component of f is independent of 2θ, a consideration of equation (9) shows that the linear absorption coefficient vanishes only for the α branch of the σ state of polarization at the point A (Fig. 6).

Discussion

Some of the more important aspects of dynamical diffraction have been derived in terms essentially simpler and more familiar to the crystallographer, without comprising rigor. It seems clear that all of its features may be treated in terms of the Darwin difference equations here described. In addition to its greater simplicity, the Darwin theory appears to be more flexible than that of Ewald and von Laue. Like band theory, the property of perfect periodicity is so fundamental to the Ewald treatment that it becomes extremely difficult to treat small deviations therefrom. For example, the propagation of either electrons or electromagnetic waves in a disordered alloy is an extremely difficult phenomenon to describe in terms of Bloch functions or the Ewald dynamical theory. But for the Darwin theory, only a relatively minor modification of the single-plane Fresnel diffraction equations is all that is required. The Borrmann effect for diffraction from a superstructure reflection of an alloy with partial long range order may as well be treated in a straightforward way with Darwin theory, while with the Ewald treatment it seems to this writer that there would be rather formidable difficulties. The possibility of an electronic analog to Darwin dynamical theory is interesting.

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