

5.1. DYNAMICAL THEORY OF X-RAY DIFFRACTION

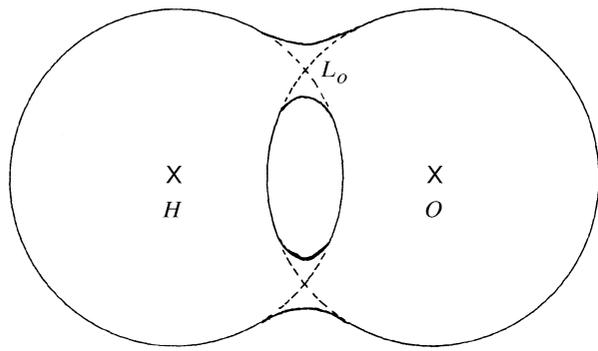


Fig. 5.1.2.3. Intersection of the dispersion surface with the plane of incidence. The dispersion surface is a connecting surface between the two spheres centred at reciprocal-lattice points O and H and with radius nk . L_o is the Lorentz point.

propagate in the crystal with a given frequency. This locus is called the *dispersion surface*. It is a constant-energy surface and is the equivalent of the index surface in optics. It is the X-ray analogue of the constant-energy surfaces known as Fermi surfaces in the electron band theory of solids.

In the two-beam case, the dispersion surface is a surface of revolution around the diffraction vector \mathbf{OH} . It is made from two spheres and a connecting surface between them. The two spheres are centred at O and H and have the same radius, nk . Fig. 5.1.2.3 shows the intersection of the dispersion surface with a plane passing through \mathbf{OH} . When the tie point lies on one of the two spheres, far from their intersection, only one wavefield propagates inside the crystal. When it lies on the connecting surface, two waves are excited simultaneously. The equation of this surface is obtained by equating to zero the determinant of system (5.1.2.20):

$$X_o X_h = k^2 C^2 \chi_h \chi_{\bar{h}} / 4. \quad (5.1.2.22)$$

Equations (5.1.2.21) show that, in the zero-absorption case, X_o and X_h are to be interpreted as the distances of the tie point P from the spheres centred at O and H , respectively. From (5.1.2.20) it can be seen that they are of the order of the vacuum wavenumber times the Fourier coefficient of the dielectric susceptibility, that is five or six orders of magnitude smaller than k . The two spheres can therefore be replaced by their tangential planes. Equation (5.1.2.22) shows that the product of the distances of the tie point from these planes is constant. The intersection of the dispersion surface with the plane passing through \mathbf{OH} is therefore a hyperbola (Fig. 5.1.2.4) whose diameter [using (5.1.2.5) and (5.1.2.22)] is

$$\overline{A_{o2}A_{o1}} = |C|R\lambda(F_h F_{\bar{h}})^{1/2} / (\pi V \cos \theta). \quad (5.1.2.23)$$

It can be noted that the larger the diameter of the dispersion surface, the larger the structure factor, that is, the stronger the interaction of the waves with the matter. When the polarization is parallel to the plane of incidence ($C = \cos 2\theta$), the interaction is weaker.

The asymptotes T_o and T_h to the hyperbola are tangents to the circles centred at O and H , respectively. Their intersection, L_o , is called the *Lorentz point* (Fig. 5.1.2.4).

A wavefield propagating in the crystal is characterized by a tie point P on the dispersion surface and two waves with wavevectors $\mathbf{K}_o = \mathbf{OP}$ and $\mathbf{K}_h = \mathbf{HP}$, respectively. The ratio, ξ , of their amplitudes D_h and D_o is given by means of (5.1.2.20):

$$\xi = \frac{D_h}{D_o} = \frac{2X_o}{kC\chi_{\bar{h}}} = \frac{-2\pi V X_o}{R\lambda C F_{\bar{h}}}. \quad (5.1.2.24)$$

The hyperbola has two branches, 1 and 2, for each direction of polarization, that is, for $C = 1$ or $\cos 2\theta$ (Fig. 5.1.2.5). Branch 2 is

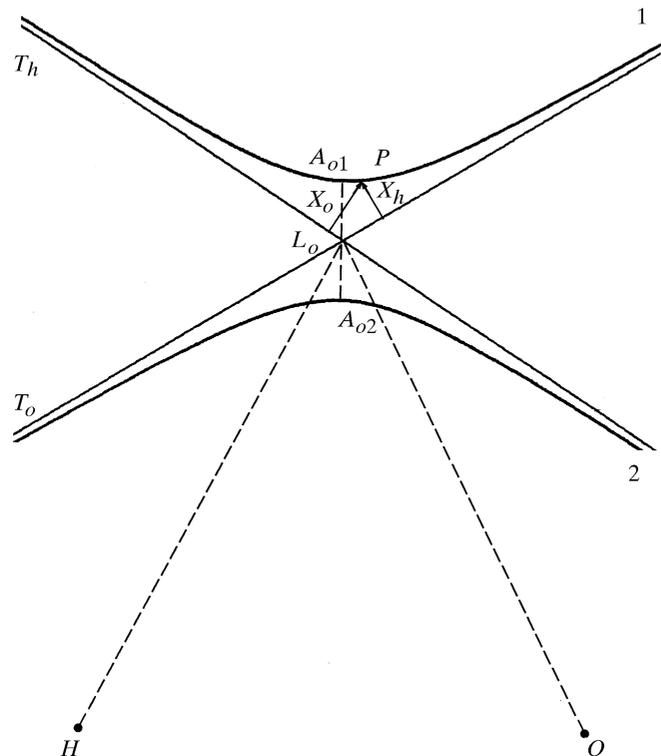


Fig. 5.1.2.4. Intersection of the dispersion surface with the plane of incidence shown in greater detail. The Lorentz point L_o is far away from the nodes O and H of the reciprocal lattice: $OL_o = HL_o = 1/\lambda$ is about 10^5 to 10^6 times larger than the diameter $A_{o1}A_{o2}$ of the dispersion surface.

the one situated on the same side of the asymptotes as the reciprocal-lattice points O and H . Given the orientation of the wavevectors, which has been chosen away from the reciprocal-lattice points (Fig. 5.1.2.1b), the coordinates of the tie point, X_o and X_h , are positive for branch 1 and negative for branch 2. The phase of ξ is therefore equal to $\pi + \varphi_h$ and to φ_h for the two branches, respectively, where φ_h is the phase of the structure factor [equation (5.1.2.6)]. This difference of π between the two branches has important consequences for the properties of the wavefields.

As mentioned above, owing to absorption, wavevectors are actually complex and so is the dispersion surface.

5.1.2.6. Propagation direction

The energy of all the waves in a given wavefield propagates in a common direction, which is obtained by calculating either the group velocity or the Poynting vector [see Section A5.1.1.4, equation (A5.1.1.8) of the Appendix]. It can be shown that, averaged over time and the unit cell, the Poynting vector of a wavefield is

$$\mathbf{S} = (c/\varepsilon_0) \exp(4\pi\mathbf{K}_{oi} \cdot \mathbf{r}) \left[|D_o|^2 \mathbf{s}_o + |D_h|^2 \mathbf{s}_h \right], \quad (5.1.2.25)$$

where \mathbf{s}_o and \mathbf{s}_h are unit vectors in the \mathbf{K}_o and \mathbf{K}_h directions, respectively, c is the velocity of light and ε_0 is the dielectric permittivity of a vacuum. This result was first shown by von Laue (1952) in the two-beam case and was generalized to the n -beam case by Kato (1958).

From (5.1.2.25) and equation (5.1.2.22) of the dispersion surface, it can be shown that the propagation direction of the wavefield lies along the normal to the dispersion surface at the tie point (Fig. 5.1.2.5). This result is also obtained by considering the group velocity of the wavefield (Ewald, 1958; Wagner, 1959). The angle α