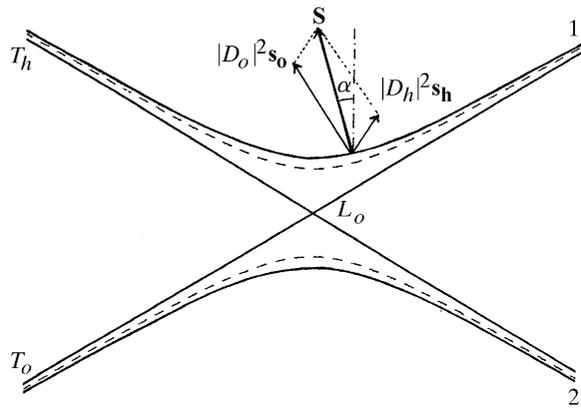## 5. DYNAMICAL THEORY AND ITS APPLICATIONS

Fig. 5.1.2.5. Dispersion surface for the two states of polarization. Solid curve: polarization normal to the plane of incidence ($C = 1$); broken curve: polarization parallel to the plane of incidence ($C = \cos 2\theta$). The direction of propagation of the energy of the wavefields is along the Poynting vector, **S**, normal to the dispersion surface.

between the propagation direction and the lattice planes is given by

$$\tan \alpha = \left[(1 - |\xi|^2)/(1 + |\xi|^2) \right] \tan \theta. \qquad (5.1.2.26)$$

It should be noted that the propagation direction varies between $\mathbf{K_o}$ and $\mathbf{K_h}$ for both branches of the dispersion surface.

5.1.3. Solutions of plane-wave dynamical theory

5.1.3.1. *Departure from Bragg's law of the incident wave*

The wavefields excited in the crystal by the incident wave are determined by applying the boundary condition mentioned above for the continuity of the tangential component of the wavevectors (Section 5.1.2.3). Waves propagating in a vacuum have wavenumber $k = 1/\lambda$. Depending on whether they propagate in the incident or in the reflected direction, the common extremity, M, of their wavevectors

$$\mathbf{OM} = \mathbf{K_o}^{(a)} \text{ and } \mathbf{HM} = \mathbf{K_h}^{(a)}$$

lies on spheres of radius k and centred at O and H, respectively. The intersections of these spheres with the plane of incidence are two circles which can be approximated by their tangents T_o' and T_h' at their intersection point, L_a, or *Laue point* (Fig. 5.1.3.1).
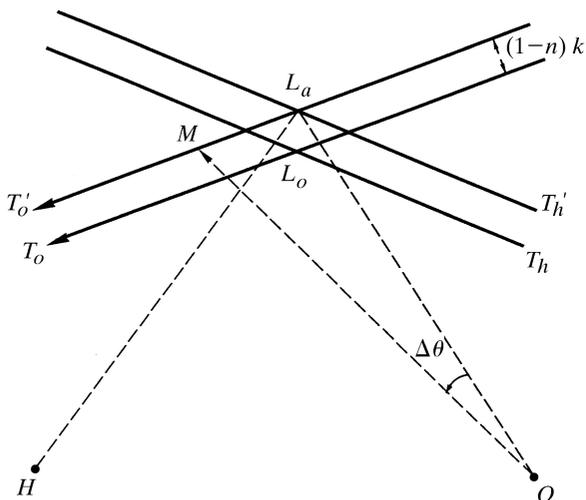

Fig. 5.1.3.1. Departure from Bragg's law of an incident wave.

Bragg's condition is exactly satisfied according to the geometrical theory of diffraction when M lies at L_a. The departure $\Delta\theta$ from Bragg's incidence of an incident wave is defined as the angle between the corresponding wavevectors **OM** and $\mathbf{OL}_a$. As $\Delta\theta$ is very small compared to the Bragg angle in the general case of X-rays or neutrons, one may write

$$\mathbf{K_o}^{(a)} = \mathbf{OM} = \mathbf{OL}_a + \mathbf{L}_a\mathbf{M},$$
$$\Delta\theta = \overline{L_aM}/k. \qquad (5.1.3.1)$$

The tangent T_o' is oriented in such a way that $\Delta\theta$ is negative when the angle of incidence is smaller than the Bragg angle.

5.1.3.2. *Transmission and reflection geometries*

The boundary condition for the continuity of the tangential component of the wavevectors is applied by drawing from M a line, **Mz**, parallel to the normal **n** to the crystal surface. The tie points of the wavefields excited in the crystal by the incident wave are at the intersections of this line with the dispersion surface. Two different situations may occur:

(*a*) *Transmission, or Laue case* (Fig. 5.1.3.2). The normal to the crystal surface drawn from M intersects *both* branches of the dispersion surface (Fig. 5.1.3.2*a*). The reflected wave is then directed towards the *inside* of the crystal (Fig. 5.1.3.2*b*). Let γ_o and γ_h be the cosines of the angles between the normal to the crystal surface, **n**, and the incident and reflected directions, respectively:
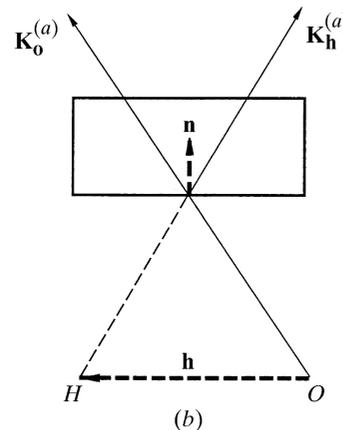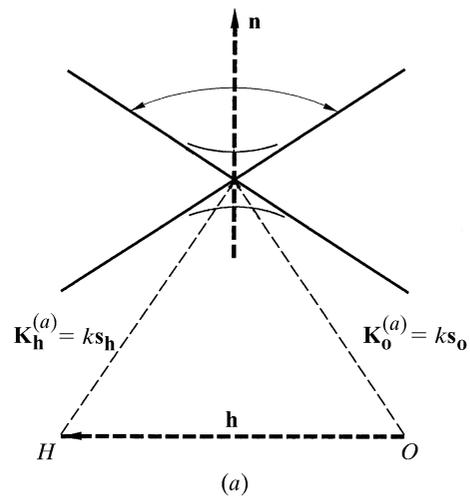

(*a*)

(*b*)

Fig. 5.1.3.2. Transmission, or Laue, geometry. (*a*) Reciprocal space; (*b*) direct space.

references