International Tables for Crystallography (2006). Vol. B, Section 5.1.3.2, pp. 538–539.

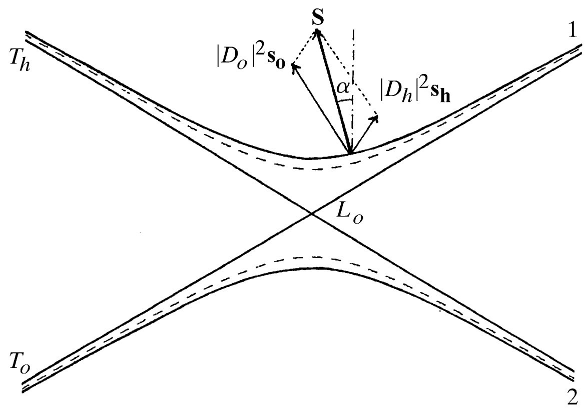

Fig. 5.1.2.5. Dispersion surface for the two states of polarization. Solid curve: polarization normal to the plane of incidence ($C = 1$); broken curve: polarization parallel to the plane of incidence ($C = \cos 2\theta$). The direction of propagation of the energy of the wavefields is along the Poynting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

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

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).

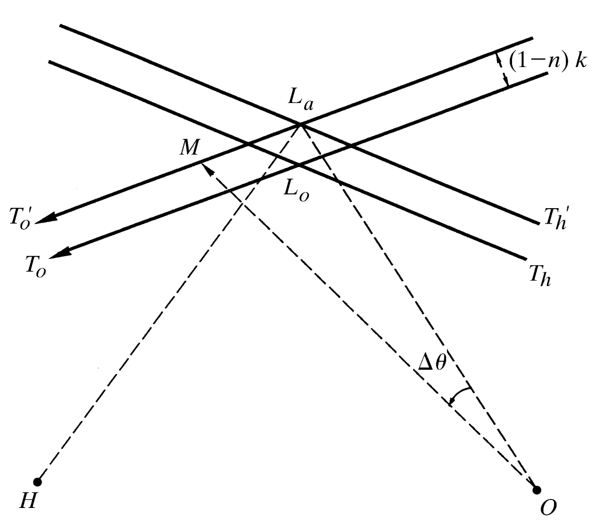

Fig. 5.1.3.1. Departure from Bragg's law of an incident wave.

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

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

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:

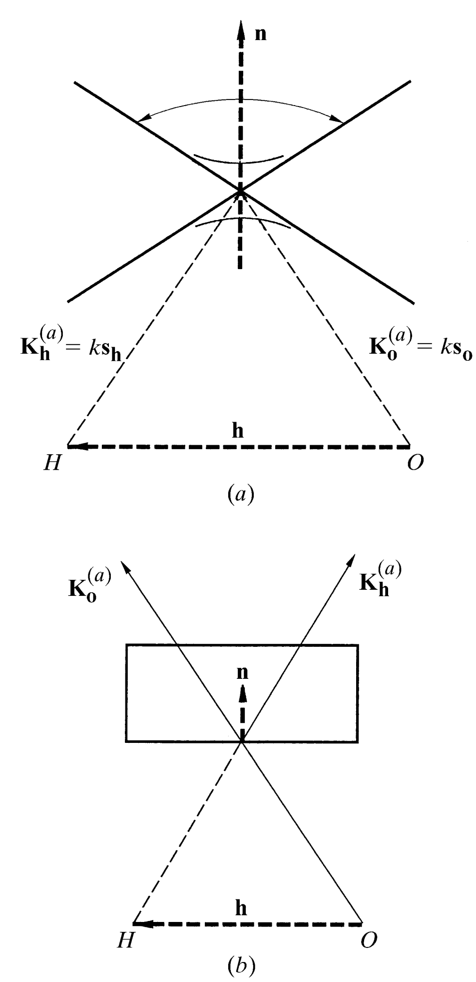

Fig. 5.1.3.2. Transmission, or Laue, geometry. (*a*) Reciprocal space; (*b*) direct space.

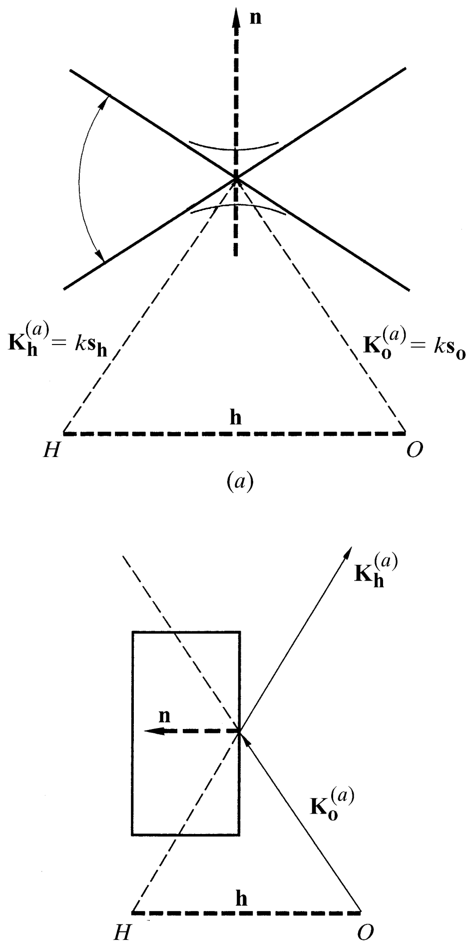

Fig. 5.1.3.3. Reflection, or Bragg, geometry. (*a*) Reciprocal space; (*b*) direct space.

$$\gamma_o = \cos(\mathbf{n}, \mathbf{s_o}); \quad \gamma_h = \cos(\mathbf{n}, \mathbf{s_h}). \tag{5.1.3.2}$$

It will be noted that they are both positive, as is their ratio,

$$\gamma = \gamma_h / \gamma_o. \tag{5.1.3.3}$$

This is the *asymmetry ratio*, which is very important since the width of the rocking curve is proportional to its square root [equation (5.1.3.6)].

(*b*) *Reflection, or Bragg case* (Fig. 5.1.3.3). In this case there are three possible situations: the normal to the crystal surface drawn from M intersects either branch 1 or branch 2 of the dispersion surface, or the intersection points are imaginary (Fig. 5.1.3.3*a*). The reflected wave is directed towards the *outside* of the crystal (Fig. 5.1.3.3*b*). The cosines defined by (5.1.3.2) are now positive for γ_o and negative for γ_h. The asymmetry factor is therefore also negative.

5.1.3.3. *Middle of the reflection domain*

It will be apparent from the equations given later that the incident wavevector corresponding to the middle of the reflection domain is, in both cases, **OI**, where I is the intersection of the normal to the crystal surface drawn from the Lorentz point, L_o, with T'_o (Figs. 5.1.3.4 and 5.1.3.5), while, according to Bragg's law, it should be $\mathbf{OL}_a$. The angle $\Delta\theta$ between the incident wavevectors $\mathbf{OL}_a$ and **OI**, corresponding to the middle of the reflecting domain according to the geometrical and dynamical theories, respectively, is

$$\Delta\theta_o = \overline{L_a I}/k = R\lambda^2 F_o (1-\gamma)/(2\pi V \sin 2\theta). \tag{5.1.3.4}$$

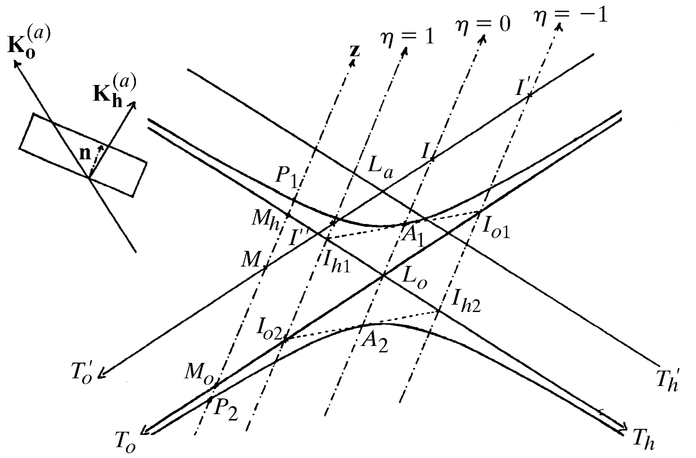

Fig. 5.1.3.4. Boundary conditions at the entrance surface for transmission geometry.

In the Bragg case, the asymmetry ratio γ is negative and $\Delta\theta_o$ is never equal to zero. This difference in Bragg angle between the two theories is due to the refraction effect, which is neglected in geometrical theory. In the Laue case, $\Delta\theta_o$ is equal to zero for symmetric reflections ($\gamma = 1$).

5.1.3.4. *Deviation parameter*

The solutions of dynamical theory are best described by introducing a reduced parameter called the *deviation parameter*,

$$\eta = (\Delta\theta - \Delta\theta_o)/\delta, \tag{5.1.3.5}$$

where

$$\delta = R\lambda^2 |C| (|\gamma| F_h F_{\bar{h}})^{1/2} / (\pi V \sin 2\theta), \tag{5.1.3.6}$$

whose real part is equal to the half width of the rocking curve (Sections 5.1.6 and 5.1.7). The width 2δ of the rocking curve is sometimes called the *Darwin width*.

The definition (5.1.3.5) of the deviation parameter is independent of the geometrical situation (reflection or transmission case); this is not followed by some authors. The present convention has the advantage of being quite general.

In an absorbing crystal, $\eta, \Delta\theta_o$ and δ are complex, and it is the real part, $\Delta\theta_{or}$, of $\Delta\theta_o$ which has the geometrical interpretation given in Section 5.1.3.3. One obtains

$$\begin{aligned} &\eta = \eta_r + i\eta_i \\ &\eta_r = (\Delta\theta - \Delta\theta_{or})/\delta_r; \ \eta_i = A\eta_r + B \\ &A = -\tan\beta \\ &B = \left\{\chi_{io} / \left[|C| (|\chi_h \chi_{\bar{h}}|)^{1/2} \cos\beta\right]\right\} (1-\gamma)/2(|\gamma|)^{1/2}, \end{aligned} \tag{5.1.3.7}$$

where β is the phase angle of $(\chi_h \chi_{\bar{h}})^{1/2}$ [or that of $(F_h F_{\bar{h}})^{1/2}$].

5.1.3.5. *Pendellösung and extinction distances*

Let

$$\Lambda_o = \pi V (\gamma_o |\gamma_h|)^{1/2} / [R\lambda |C| (F_h F_{\bar{h}})^{1/2}]. \tag{5.1.3.8}$$

This length plays a very important role in the dynamical theory of diffraction by both perfect and deformed crystals. For example, it is 15.3 µm for the 220 reflection of silicon, with Mo $K\alpha$ radiation and a symmetric reflection.

In *transmission* geometry, it gives the period of the interference between the two excited wavefields which constitutes the *Pendellösung* effect first described by Ewald (1917) (see Section

references