International Tables for Crystallography (2006). Vol. B, Figure 5.1.3.3, p. 539.

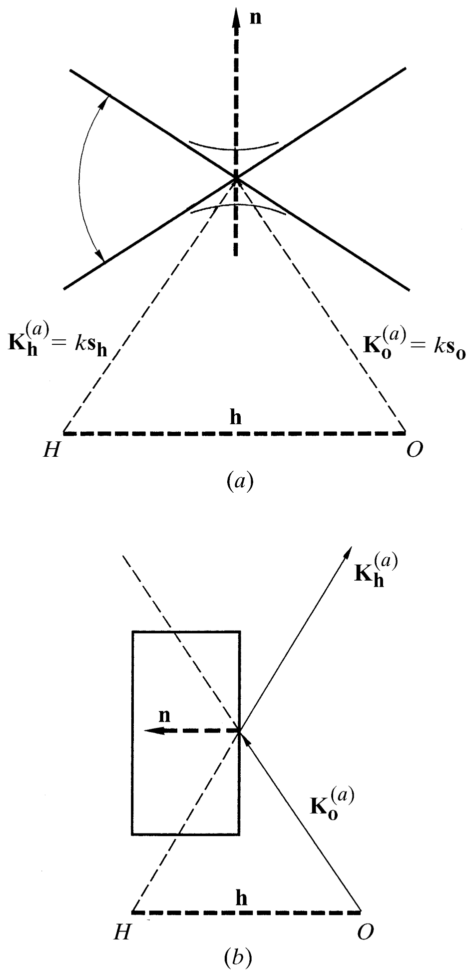

Fig. 5.1.3.3. Reflection, or Bragg, geometry. (*a*) Reciprocal space; (*b*) direct space.

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

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

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

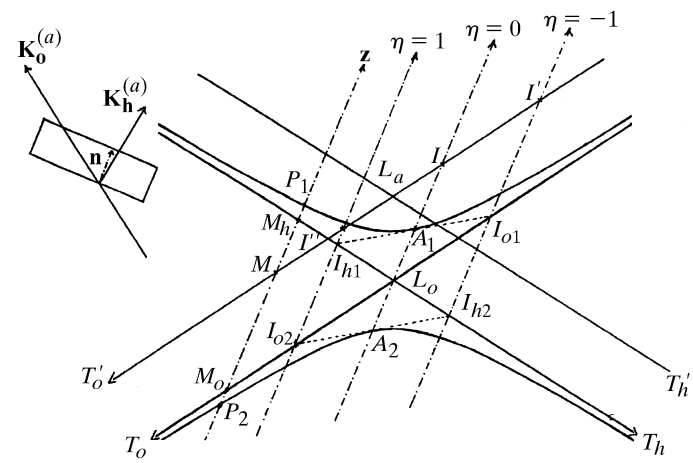

Fig. 5.1.3.4. Boundary conditions at the entrance surface for transmission geometry.

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