

5.1. DYNAMICAL THEORY OF X-RAY DIFFRACTION

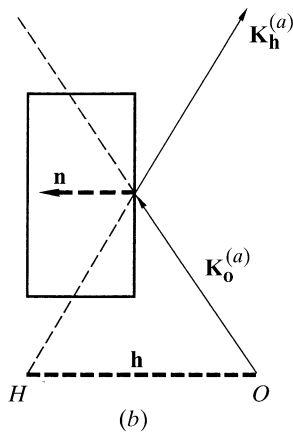
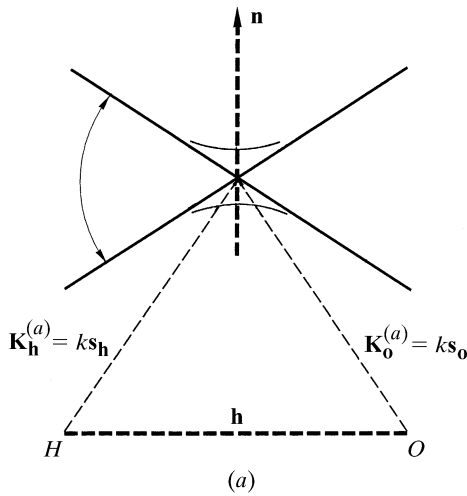


Fig. 5.1.3.3. Reflection, or Bragg, geometry. (a) Reciprocal space; (b) direct space.

$$\gamma_o = \cos(\mathbf{n}, \mathbf{s}_o); \quad \gamma_h = \cos(\mathbf{n}, \mathbf{s}_h). \quad (5.1.3.2)$$

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

$$\gamma = \gamma_h / \gamma_o. \quad (5.1.3.3)$$

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. 5.1.3.3a). The reflected wave is directed towards the *outside* of the crystal (Fig. 5.1.3.3b). 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, \mathbf{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 \mathbf{OI} , corresponding to the middle of the reflecting domain according to the geometrical and dynamical theories, respectively, is

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

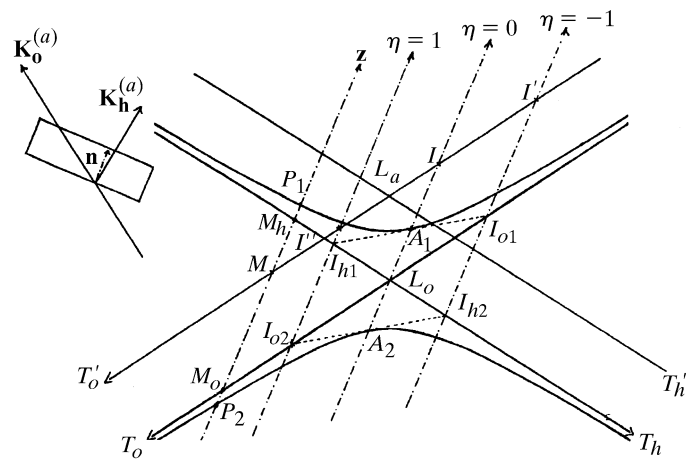


Fig. 5.1.3.4. Boundary conditions at the entrance surface for transmission geometry.

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*,

$$\eta = (\Delta\theta - \Delta\theta_o) / \delta, \quad (5.1.3.5)$$

where

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

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, η , $\Delta\theta_o$ 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

$$\begin{aligned} \eta &= \eta_r + i\eta_i \\ \eta_r &= (\Delta\theta - \Delta\theta_{or}) / \delta_r; \quad \eta_i = A\eta_r + B \end{aligned} \quad (5.1.3.7)$$

$$\begin{aligned} A &= -\tan \beta \\ B &= \left\{ \chi_{io} / \left[|C| (|\chi_h \chi_{\bar{h}}|)^{1/2} \cos \beta \right] \right\} (1 - \gamma) / 2 (|\gamma|)^{1/2}, \end{aligned}$$

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

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

This length plays a very important role in the dynamical theory of diffraction by both perfect and deformed crystals. For example, it is $15.3 \mu\text{m}$ 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