International Tables for Crystallography (2006). Vol. B, Section 5.1.3.5, pp. 539–540.

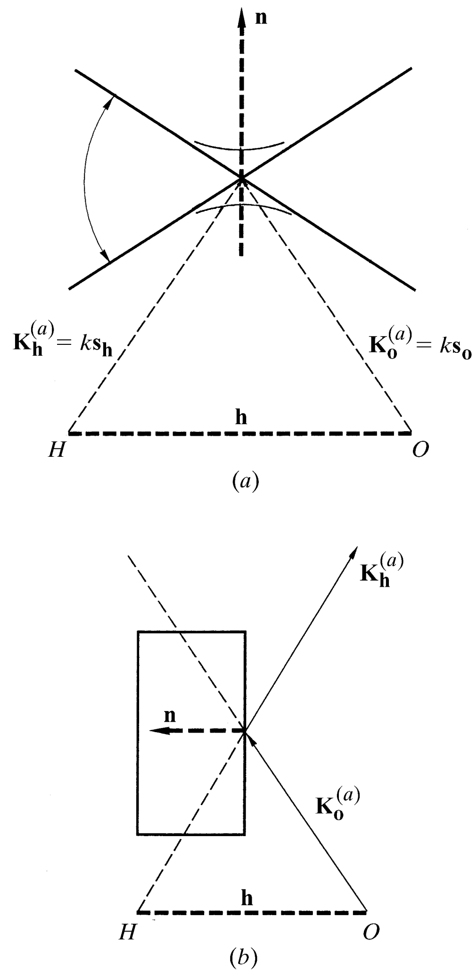

Fig. 5.1.3.3. Reflection, or Bragg, geometry. (*a*) Reciprocal space; (*b*) direct space.

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

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

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

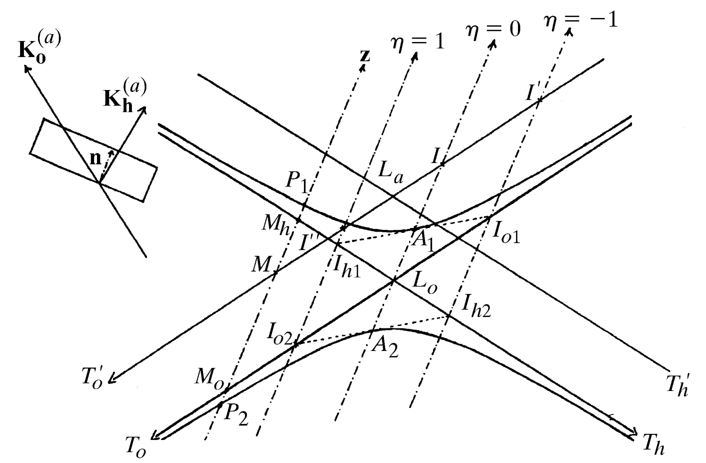

Fig. 5.1.3.4. Boundary conditions at the entrance surface for transmission geometry.

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

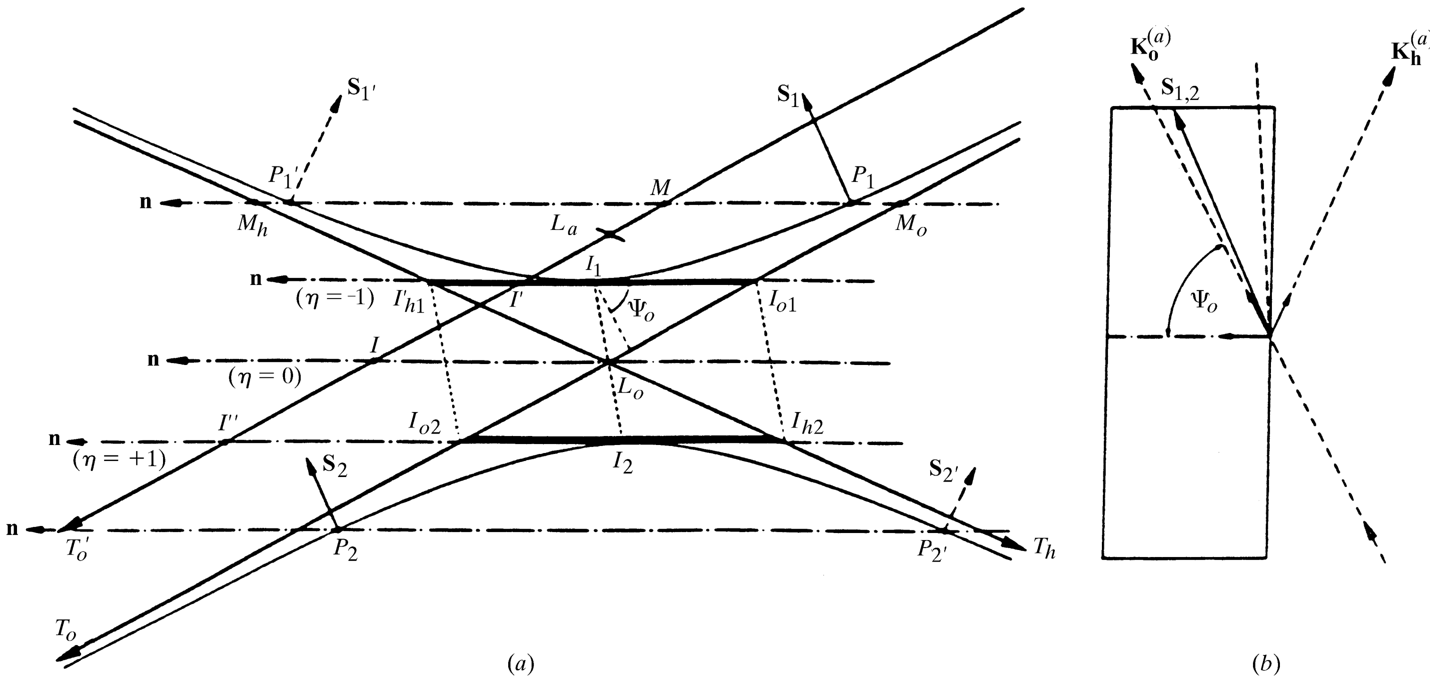

Fig. 5.1.3.5. Boundary conditions at the entrance surface for reflection geometry. (*a*) Reciprocal space; (*b*) direct space.

5.1.6.3); Λ_o in this case is called the *Pendellösung distance*, denoted Λ_L hereafter. Its geometrical interpretation, in the zero-absorption case, is the inverse of the diameter A_2A_1 of the dispersion surface in a direction defined by the cosines γ_h and γ_o with respect to the reflected and incident directions, respectively (Fig. 5.1.3.4). It reduces to the inverse of $A_{o2}A_{o1}$ (5.1.2.23) in the symmetric case.

In *reflection* geometry, it gives the absorption distance in the total-reflection domain and is called the *extinction* distance, denoted Λ_B (see Section 5.1.7.1). Its geometrical interpretation in the zero-absorption case is the inverse of the length $I_{o1}I_{h1} = I_{h2}I_{o2}$, Fig. 5.1.3.5.

In a *deformed* crystal, if distortions are of the order of the width of the rocking curve over a distance Λ_o, the crystal is considered to be slightly deformed, and ray theory (Penning & Polder, 1961; Kato, 1963, 1964*a*,*b*) can be used to describe the propagation of wavefields. If the distortions are larger, new wavefields may be generated by interbranch scattering (Authier & Balibar, 1970) and generalized dynamical diffraction theory such as that developed by Takagi (1962, 1969) should be used.

Using (5.1.3.8), expressions (5.1.3.5) and (5.1.3.6) can be rewritten in the very useful form:

$$\begin{aligned}\eta &= (\Delta\theta - \Delta\theta_o)\Lambda_o \sin 2\theta/(\lambda|\gamma_h|),\\ \delta &= \lambda|\gamma_h|/(\Lambda_o \sin 2\theta).\end{aligned} \qquad (5.1.3.9)$$

The order of magnitude of the Darwin width 2δ ranges from a fraction of a second of an arc to ten or more seconds, and increases with increasing wavelength and increasing structure factor. For example, for the 220 reflection of silicon and Cu $K\alpha$ radiation, it is 5.2 seconds.

5.1.3.6. *Solution of the dynamical theory*

The coordinates of the tie points excited by the incident wave are obtained by looking for the intersection of the dispersion surface, (5.1.2.22), with the normal **Mz** to the crystal surface (Figs. 5.1.3.4 and 5.1.3.5). The ratio ξ of the amplitudes of the waves of the corresponding wavefields is related to these coordinates by (5.1.2.24) and is found to be

$$\begin{aligned}\xi_j &= D_{hj}/D_{oj}\\ &= -S(C)S(\gamma_h)[(F_hF_{\bar h})^{1/2}/F_{\bar h}]\\ &\quad\times \left\{\eta \pm \left[\eta^2 + S(\gamma_h)\right]^{1/2}\right\}/(|\gamma|)^{1/2},\end{aligned} \qquad (5.1.3.10)$$

where the plus sign corresponds to a tie point on branch 1 ($j = 1$) and the minus sign to a tie point on branch 2 ($j = 2$), and $S(\gamma_h)$ is the sign of γ_h (+1 in transmission geometry, -1 in reflection geometry).

5.1.3.7. *Geometrical interpretation of the solution in the zero-absorption case*

5.1.3.7.1. *Transmission geometry*

In this case (Fig. 5.1.3.4) $S(\gamma_h)$ is +1 and (5.1.3.10) may be written

$$\xi_j = -S(C)\left[\eta \pm (\eta^2 + 1)^{1/2}\right]/\gamma^{1/2}. \qquad (5.1.3.11)$$

Let A_1 and A_2 be the intersections of the normal to the crystal surface drawn from the Lorentz point L_o with the two branches of the dispersion surface (Fig. 5.1.3.4). From Sections 5.1.3.3 and 5.1.3.4, they are the tie points excited for $\eta = 0$ and correspond to the middle of the reflection domain. Let us further consider the tangents to the dispersion surface at A_1 and A_2 and let I_{o1}, I_{o2} and I_{h1}, I_{h2} be their intersections with T_o and T_h, respectively. It can be shown that $\overline{I_{o1}I_{h2}}$ and $\overline{I_{o2}I_{h1}}$ intersect the dispersion surface at the tie points excited for $\eta = -1$ and $\eta = +1$, respectively, and that the *Pendellösung* distance $\Lambda_L = 1/\overline{A_2A_1}$, the width of the rocking curve $2\delta = \overline{I_{o1}I_{o2}}/k$ and the deviation parameter $\eta = \overline{M_oM_h}/\overline{A_2A_1}$, where M_o and M_h are the intersections of the normal to the crystal surface drawn from the extremity of any incident wavevector **OM** with T_o and T_h, respectively.