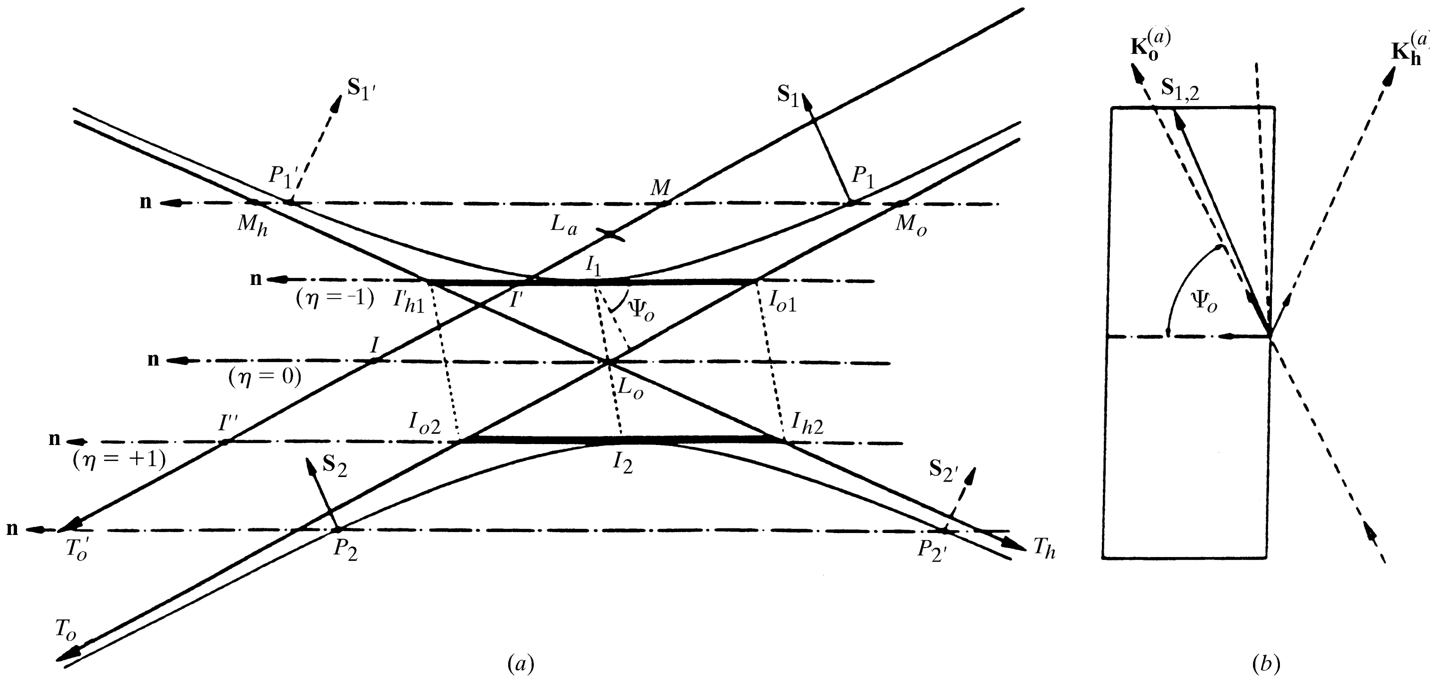

Fig. 5.1.3.5. Boundary conditions at the entrance surface for reflection geometry. (*a*) Reciprocal space; (*b*) direct space.

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

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

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 $\mathrm{S}(\gamma_h)$ 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) $\mathrm{S}(\gamma_h)$ is +1 and (5.1.3.10) may be written

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

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.

references