International Tables for Crystallography (2006). Vol. B, Section 5.1.6.4, pp. 543–544.

again the condition of the continuity of their tangential components along the crystal surface. The extremities, M_j and N_j, of these wavevectors

$$\mathbf{OM}_j = \mathbf{K}_{\mathbf{o}j}^{(d)} \qquad \mathbf{HN}_j = \mathbf{K}_{\mathbf{h}j}^{(d)}$$

lie at the intersections of the spheres of radius k centred at O and H, respectively, with the normal $\mathbf{n}'$ to the crystal exit surface drawn from P_j ($j = 1$ and 2) (Fig. 5.1.6.3).

If the crystal is wedge-shaped and the normals $\mathbf{n}$ and $\mathbf{n}'$ to the entrance and exit surfaces are not parallel, the wavevectors of the waves generated by the two wavefields are not parallel. This effect is due to the refraction properties associated with the dispersion surface.

5.1.6.3.2. *Amplitudes – Pendellösung*

We shall assume from now on that the crystal is plane parallel. Two wavefields arrive at any point of the exit surface. Their constituent waves interfere and generate emerging waves in the refracted and reflected directions (Fig. 5.1.6.4). Their respective amplitudes are given by the boundary conditions

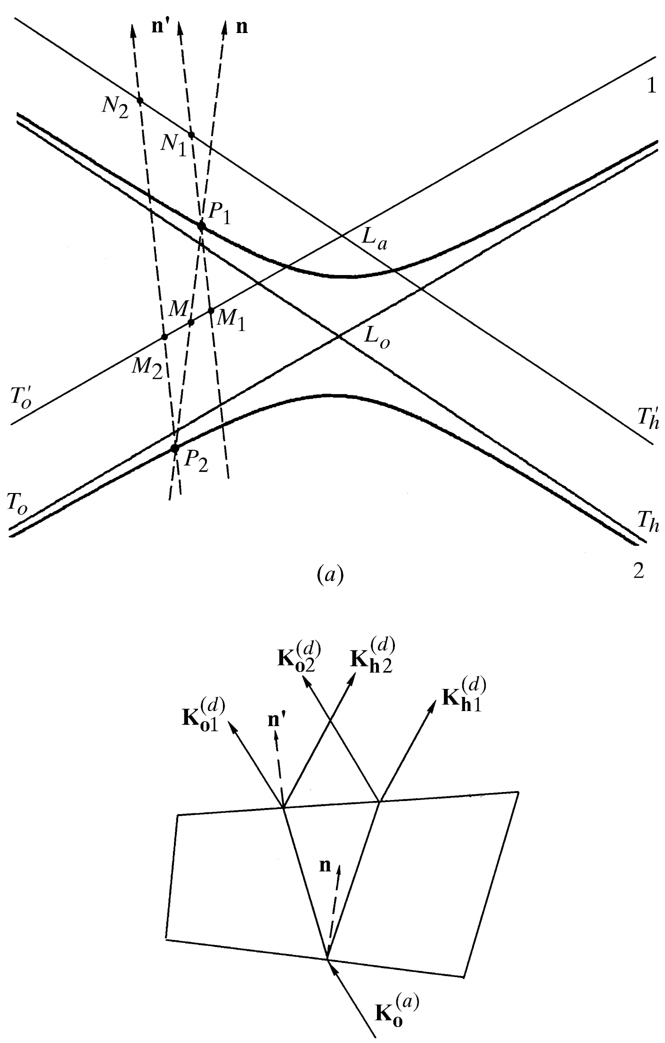

Fig. 5.1.6.3. Boundary condition for the wavevectors at the exit surface. (*a*) Reciprocal space. The wavevectors of the emerging waves are determined by the intersections M_1, M_2, N_1 and N_2 of the normals $\mathbf{n}'$ to the exit surface, drawn from the tie points P_1 and P_2 of the wavefields, with the tangents T_o' and T_h' to the spheres centred at O and H and of radius k, respectively. (*b*) Direct space.

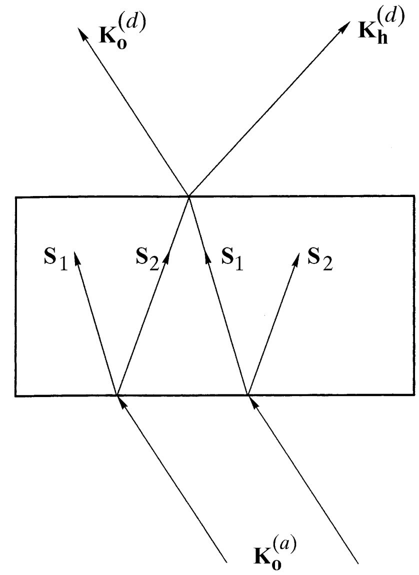

Fig. 5.1.6.4. Decomposition of a wavefield into its two components when it reaches the exit surface. $\mathbf{S}_1$ and $\mathbf{S}_2$ are the Poynting vectors of the two wavefields propagating in the crystal belonging to branches 1 and 2 of the dispersion surface, respectively, and interfering at the exit surface.

$$\begin{aligned} D_o^{(d)} \exp(-2\pi i \mathbf{K}_\mathbf{o}^{(d)} \cdot \mathbf{r}) &= D_{o1} \exp(-2\pi i \mathbf{K}_{\mathbf{o}1} \cdot \mathbf{r}) \\ &\quad + D_{o2} \exp(-2\pi i \mathbf{K}_{\mathbf{o}2} \cdot \mathbf{r}) \\ D_h^{(d)} \exp(-2\pi i \mathbf{K}_\mathbf{h}^{(d)} \cdot \mathbf{r}) &= D_{h1} \exp(-2\pi i \mathbf{K}_{\mathbf{h}1} \cdot \mathbf{r}) \\ &\quad + D_{h2} \exp(-2\pi i \mathbf{K}_{\mathbf{h}2} \cdot \mathbf{r}), \end{aligned} \tag{5.1.6.4}$$

where $\mathbf{r}$ is the position vector of a point on the exit surface, the origin of phases being taken at the entrance surface.

In a plane-parallel crystal, (5.1.6.4) reduces to

$$\begin{aligned} D_o^{(d)} &= D_{o1} \exp\big(-2\pi i \overline{MP_1} \cdot t\big) + D_{o2} \exp\big(-2\pi i \overline{MP_2} \cdot t\big) \\ D_h^{(d)} &= D_{h1} \exp\big(-2\pi i \overline{MP_1} \cdot t\big) + D_{h2} \exp\big(-2\pi i \overline{MP_2} \cdot t\big), \end{aligned}$$

where t is the crystal thickness.

In a *non-absorbing* crystal, the amplitudes squared are of the form

$$\big|D_o^{(d)}\big|^2 = |D_{o1}|^2 + |D_{o2}|^2 + 2D_{o1}D_{o2} \cos 2\pi \overline{P_2P_1} t.$$

This expression shows that the intensities of the refracted and reflected beams are oscillating functions of crystal thickness. The period of the oscillations is called the *Pendellösung* distance and is

$$\Lambda = 1/\overline{P_2P_1} = \Lambda_L/(1 + \eta_r^2)^{1/2}.$$

5.1.6.4. *Reflecting power*

For an *absorbing* crystal, the intensities of the reflected and refracted waves are

$$\begin{aligned} \big|D_o^{(d)}\big|^2 &= \big|D_o^{(a)}\big|^2 A_\eta \Big\{ \cosh(2v + \mu_a t). \\ &\quad + \cos\Big[2\pi t \Lambda^{-1} - 2\eta_i (1 + \eta_r^2)^{-1/2}\Big] \Big\} \\ \Big|D_h^{(d)}\Big|^2 &= \big|D_o^{(a)}\big|^2 |F_h/F_{\bar{h}}| \gamma^{-1} A_\eta \big[\cosh(\mu_a t) - \cos(2\pi t \Lambda^{-1})\big], \end{aligned} \tag{5.1.6.5}$$

where

$$\begin{aligned}
A_\eta &= \left[\exp -\mu_o t(\gamma_o^{-1} + \gamma_h^{-1})\right]/2(1+\eta_r^2),\\
\mu_a &= \mu_j\Big[1/2(\gamma_o^{-1} - \gamma_h^{-1})\eta_r\\
&\quad + \ |C||F_{ih}/F_{io}|\cos\varphi/(\gamma_o\gamma_h)^{1/2}\Big](1+\eta_r^2)^{-1/2},\\
v &= \operatorname{arg\,sinh}\eta_r
\end{aligned}$$

and μ_j is given by equation (5.1.6.1).

Depending on the absorption coefficient, the cosine terms are more or less important relative to the hyperbolic cosine term and the oscillations due to *Pendellösung* have more or less contrast.

For a non-absorbing crystal, these expressions reduce to

$$\begin{aligned}
\left|D_o^{(d)}\right|^2 &= \left|D_o^{(a)}\right|^2\left[\frac{1+2\eta^2+\cos(2\pi t\Lambda^{-1})}{2(1+\eta_r^2)}\right],\\
\left|D_h^{(d)}\right|^2 &= \left|D_o^{(a)}\right|^2\left[\frac{1-\cos(2\pi t\Lambda^{-1})}{2\gamma(1+\eta_r^2)}\right].
\end{aligned} \qquad (5.1.6.6)$$

What is actually measured in a counter receiving the reflected or the refracted beam is the *reflecting power*, namely the ratio of the energy of the reflected or refracted beam on the one hand and the energy of the incident beam on the other. The energy of a beam is obtained by multiplying its intensity by its cross section. If l is the width of the trace of the beam on the crystal surface, the cross sections of the incident (or refracted) and reflected beams are proportional to (Fig. 5.1.6.5) $l_o = l\gamma_o$ and $l_h = l\gamma_h$, respectively.

The reflecting powers are therefore:

$$\text{Refracted beam: } I_o = l_o\left|D_o^{(d)}\right|^2\Big/l_o\left|D_o^{(a)}\right|^2 = \left|D_o^{(d)}\right|^2\Big/\left|D_o^{(a)}\right|^2,$$

$$\text{Reflected beam: } I_h = l_h\left|D_h^{(d)}\right|^2\Big/l_o\left|D_o^{(a)}\right|^2 = \gamma\left|D_h^{(d)}\right|^2\Big/\left|D_o^{(a)}\right|^2. \qquad (5.1.6.7)$$

Using (5.1.6.6), it is easy to check that $I_o + I_h = 1$ in the non-absorbing case; that is, that conservation of energy is satisfied. Equations (5.1.6.6) show that there is a periodic exchange of energy between the refracted and the reflected waves as the beam penetrates the crystal; this is why Ewald introduced the expression *Pendellösung*.

The oscillations in the rocking curve were first observed by Lefeld-Sosnowska & Malgrange (1968, 1969). Their periodicity can be used for accurate measurements of the form factor [see, for

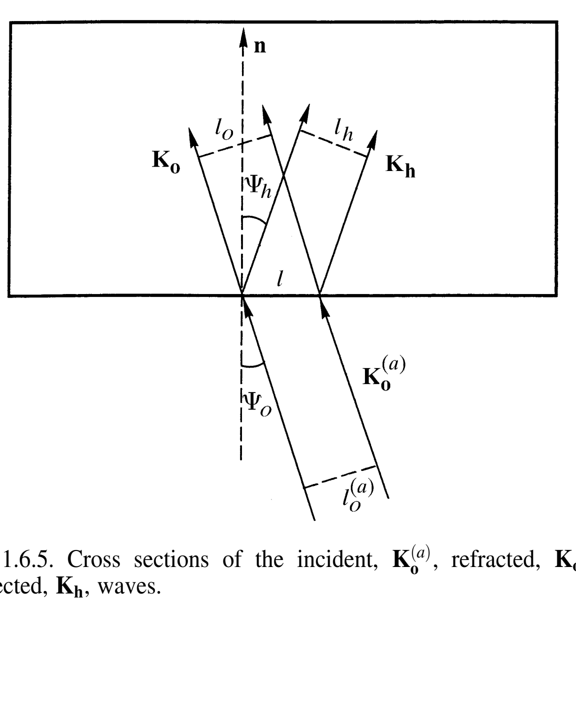

Fig. 5.1.6.5. Cross sections of the incident, $\mathbf{K_o}^{(a)}$, refracted, $\mathbf{K_o}$, and reflected, $\mathbf{K_h}$, waves.

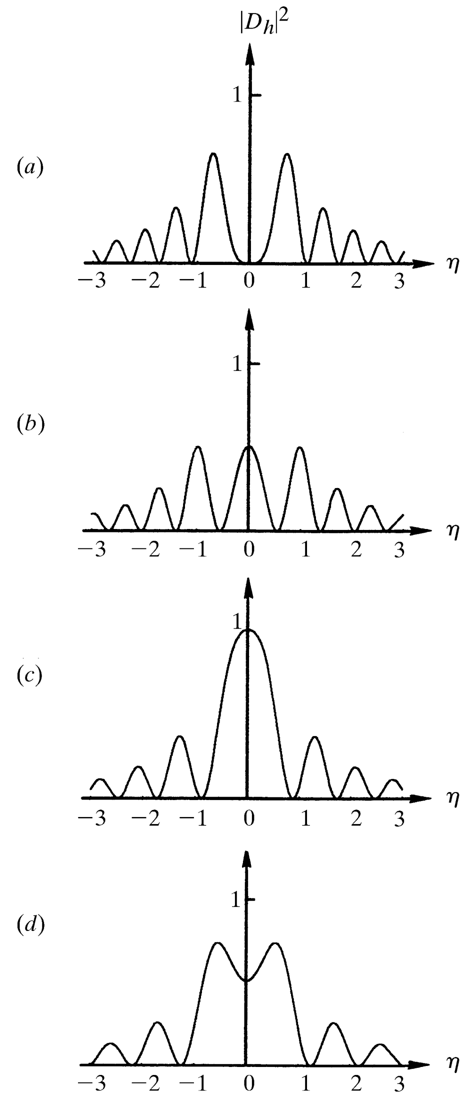

Fig. 5.1.6.6. Theoretical rocking curves in the transmission case for non-absorbing crystals and for various values of t/Λ_L: (*a*) $t/\Lambda_L = 1.25$; (*b*) $t/\Lambda_L = 1.5$; (*c*) $t/\Lambda_L = 1.75$; (*d*) $t/\Lambda_L = 2.0$.

instance, Bonse & Teworte (1980)]. Fig. 5.1.6.6 shows the shape of the rocking curve for various values of t/Λ_L.

The *width at half-height of the rocking curve*, averaged over the *Pendellösung* oscillations, corresponds in the non-absorbing case to $\Delta\eta = 2$, that is, to $\Delta\theta = 2\delta$, where δ is given by (5.1.3.6).

5.1.6.5. *Integrated intensity*

5.1.6.5.1. *Non-absorbing crystals*

The integrated intensity is the ratio of the total energy recorded in the counter when the crystal is rocked to the intensity of the incident beam. It is proportional to the area under the line profile:

$$I_{hi} = \int_{-\infty}^{+\infty} I_h \,\mathrm{d}(\Delta\theta). \qquad (5.1.6.8)$$

The integration was performed by von Laue (1960). Using (5.1.3.5), (5.1.6.6) and (5.1.6.7) gives

$$I_{hi} = A\int_0^{2\pi t\Lambda_L^{-1}} J_0(z)\,\mathrm{d}z,$$

where $J_0(z)$ is the zeroth-order Bessel function and

references