

5.1. DYNAMICAL THEORY OF X-RAY DIFFRACTION

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

$$OM_j = \mathbf{K}_{o_j}^{(d)} \quad \mathbf{HN}_j = \mathbf{K}_{h_j}^{(d)}$$

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

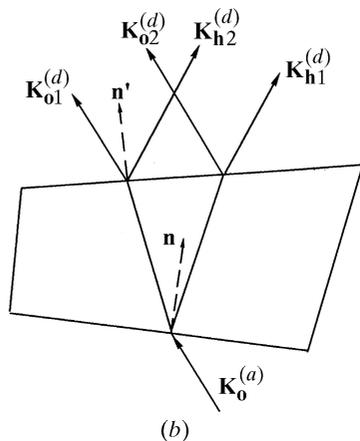
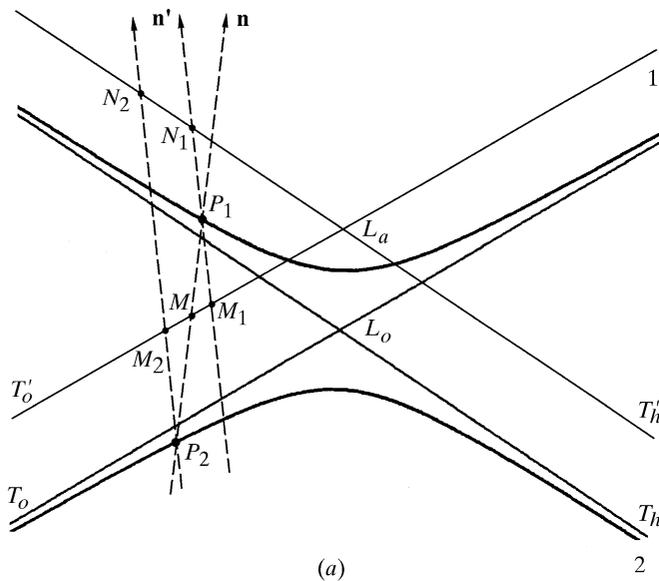


Fig. 5.1.6.3. Boundary condition for the wavevectors at the exit surface. (a) Reciprocal space. The wavevectors of the emerging waves are determined by the intersections  $M_1$ ,  $M_2$ ,  $N_1$  and  $N_2$  of the normals  $\mathbf{n}'$  to the exit surface, drawn from the tie points  $P_1$  and  $P_2$  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.

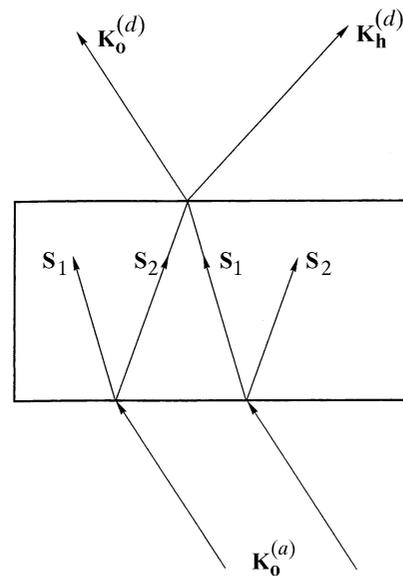


Fig. 5.1.6.4. Decomposition of a wavefield into its two components when it reaches the exit surface.  $\mathbf{S}_1$  and  $\mathbf{S}_2$  are the Poynting vectors of the two wavefields propagating in the crystal belonging to branches 1 and 2 of the dispersion surface, respectively, and interfering at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

amplitudes are given by the boundary conditions

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

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

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

where  $t$  is the crystal thickness.

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

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

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

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

where