

5. DYNAMICAL THEORY AND ITS APPLICATIONS

$$A_\eta = [\exp -\mu_o t (\gamma_o^{-1} + \gamma_h^{-1})] / 2(1 + \eta_r^2),$$

$$\mu_a = \mu_j \left[1/2(\gamma_o^{-1} - \gamma_h^{-1})\eta_r \right. \\ \left. + |C| |F_{ih}/F_{io}| \cos \varphi / (\gamma_o \gamma_h)^{1/2} \right] (1 + \eta_r^2)^{-1/2},$$

$$v = \arg \sinh \eta_r$$

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

$$|D_o^{(d)}|^2 = |D_o^{(a)}|^2 \left[\frac{1 + 2\eta^2 + \cos(2\pi t \Lambda^{-1})}{2(1 + \eta_r^2)} \right],$$

$$|D_h^{(d)}|^2 = |D_o^{(a)}|^2 \left[\frac{1 - \cos(2\pi t \Lambda^{-1})}{2\gamma(1 + \eta_r^2)} \right]. \quad (5.1.6.6)$$

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:

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

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

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

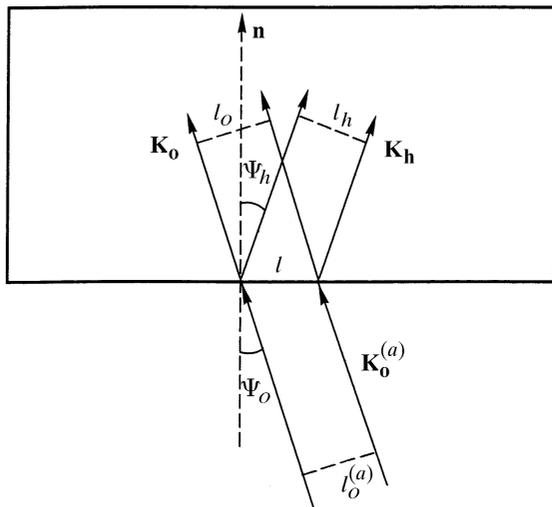


Fig. 5.1.6.5. Cross sections of the incident, $\mathbf{K}_o^{(a)}$, refracted, \mathbf{K}_o , and reflected, \mathbf{K}_h , waves.

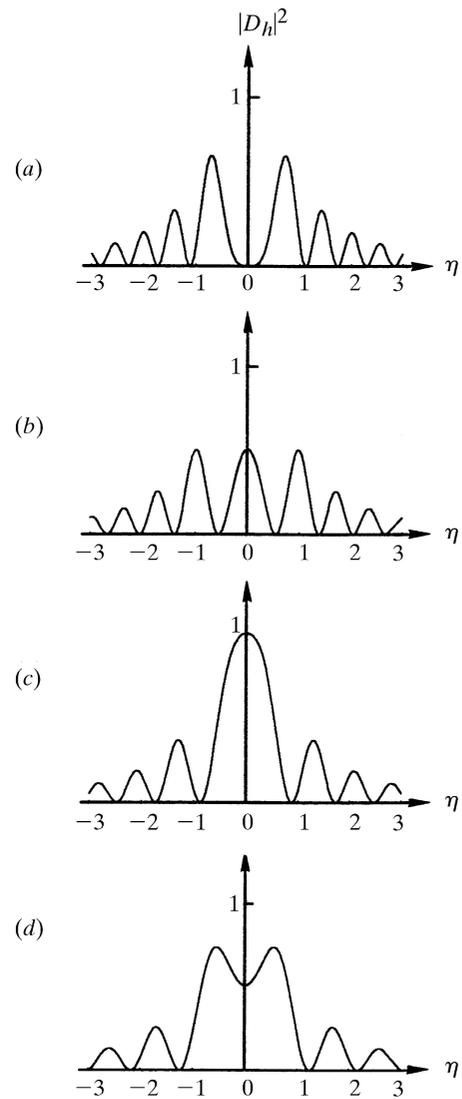


Fig. 5.1.6.6. Theoretical rocking curves in the transmission case for non-absorbing crystals and for various values of t/Λ_L : (a) $t/\Lambda_L = 1.25$; (b) $t/\Lambda_L = 1.5$; (c) $t/\Lambda_L = 1.75$; (d) $t/\Lambda_L = 2.0$.

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:

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

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

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

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