

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

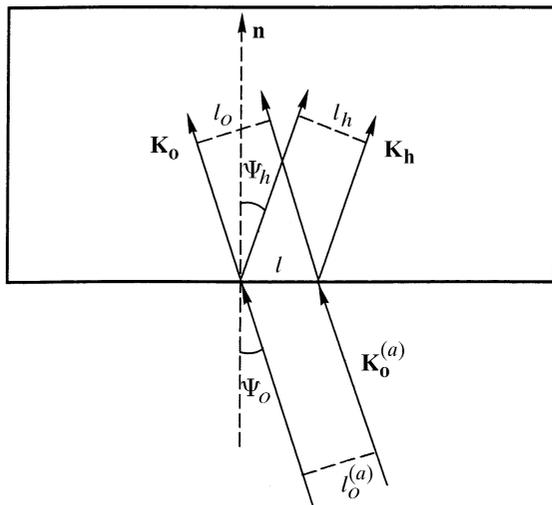


Fig. 5.1.6.5. Cross sections of the incident, $\mathbf{K}_o^{(a)}$, refracted, \mathbf{K}_o , and reflected, \mathbf{K}_h , waves.

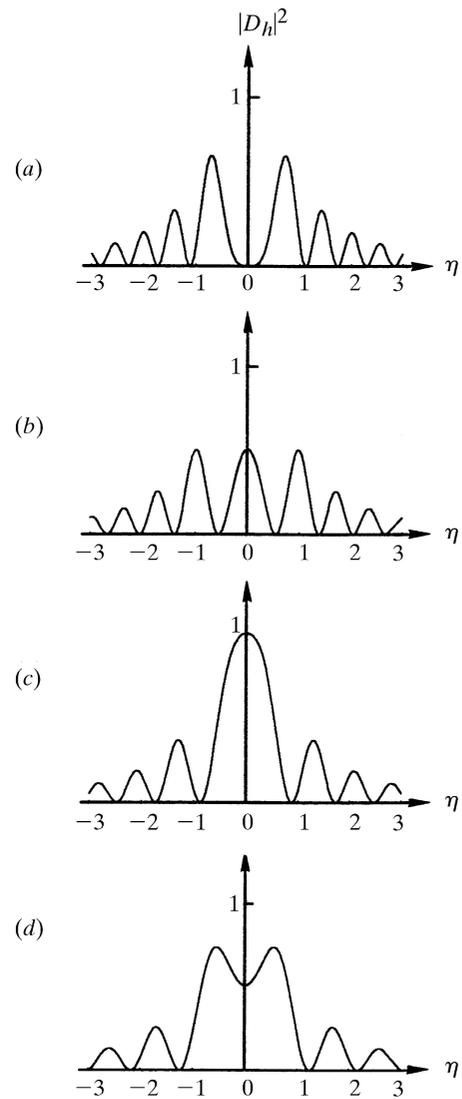


Fig. 5.1.6.6. Theoretical rocking curves in the transmission case for non-absorbing crystals and for various values of t/Λ_L : (a) $t/\Lambda_L = 1.25$; (b) $t/\Lambda_L = 1.5$; (c) $t/\Lambda_L = 1.75$; (d) $t/\Lambda_L = 2.0$.

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

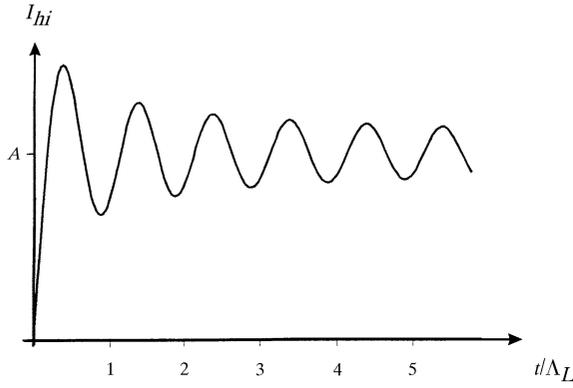


Fig. 5.1.6.7. Variations with crystal thickness of the integrated intensity in the transmission case (no absorption) (arbitrary units). The expression for A is given in the text.

$$A = \frac{R\lambda^2 |CF_h| (\gamma)^{1/2}}{2V \sin 2\theta}.$$

Fig. 5.1.6.7 shows the variations of the integrated intensity with t/Λ_L .

5.1.6.5.2. Absorbing crystals

The integration was performed for absorbing crystals by Kato (1955). The integrated intensity in this case is given by

$$I_{hi} = A |F_h/F_{\bar{h}}| \exp[-1/2\mu_o t(\gamma_o^{-1} + \gamma_h^{-1})] \times \left[\int_0^{2\pi t \Lambda_L^{-1}} J_0(z) dz - 1 + I_0(\zeta) \right],$$

where

$$\zeta = \mu_o t \left\{ \left[|C|^2 |F_{ih}/F_{io}|^2 \cos^2 \varphi + (\gamma_h - \gamma_o)/(4\gamma_o\gamma_h) \right] / (\gamma_o\gamma_h) \right\}^{1/2}$$

and $I_0(\zeta)$ is a modified Bessel function of zeroth order.

5.1.6.6. Thin crystals – comparison with geometrical theory

Using (5.1.6.6) and (5.1.6.7), the reflecting power of the reflected beam may also be written

$$I_h = \pi^2 t^2 \Lambda_o^{-2} f(\eta),$$

where

$$f(\eta) = \left[\frac{\sin U(1 + \eta^2)^{1/2}}{U(1 + \eta^2)^{1/2}} \right]^2$$

and

$$U = \pi t \Lambda_o^{-1}.$$

When $t\Lambda_o^{-1}$ is very small, $f(\eta)$ tends asymptotically towards the function

$$f_1(\eta) = \left[\frac{\sin U\eta}{U\eta} \right]^2$$

and I_h towards the value given by geometrical theory. The condition for geometrical theory to apply is, therefore, that the crystal thickness be much smaller than the *Pendellösung* distance. In practice, the two theories agree to within a few per cent for a crystal

thickness smaller than or equal to a third of the *Pendellösung* distance [see Authier & Malgrange (1998)].

5.1.7. Intensity of plane waves in reflection geometry

5.1.7.1. Thick crystals

5.1.7.1.1. Non-absorbing crystals

Rocking curve. The geometrical construction in Fig. 5.1.3.5 shows that, in the Bragg case, the normal to the crystal surface drawn from the extremity of the incident wavevector intersects the dispersion surface either at two points of the same branch, P_1, P'_1 , for branch 1, P_2, P'_2 for branch 2, or at imaginary points. It was shown in Section 5.1.2.6 that the propagation of the wavefields inside the crystal is along the normal to the dispersion surface at the corresponding tie points. Fig. 5.1.3.5 shows that this direction is oriented towards the outside of the crystal for tie points P'_1 and P'_2 . In a very thick crystal, these wavefields cannot exist because there is always a small amount of absorption. One concludes that in the thick-crystal case and in reflection geometry, only one wavefield is excited inside the crystal. It corresponds to branch 1 on the low-angle side of the rocking curve and to branch 2 on the high-angle side. Using the same approximations as in Section 5.1.6.2, the amplitude $\mathbf{D}_h^{(a)}$ of the wave reflected at the crystal surface is obtained by applying the boundary conditions, which are particularly simple in this case:

$$\mathbf{D}_o = \mathbf{D}_o^{(a)}, \quad \mathbf{D}_h^{(a)} = \mathbf{D}_h.$$

The reflecting power is given by an expression similar to (5.1.6.7):

$$I_h = |\gamma| |\xi_j|^2,$$

where the expression for ξ_j is given by (5.1.3.12), and $j = 1$ or 2 depending on which wavefield propagates towards the inside of the crystal. When the normal to the entrance surface intersects the dispersion surface at imaginary points, *i.e.* when $-1 < \eta < +1$,

$$|\xi|^2 = |\gamma|^{-1}, \quad I_h = 1, \quad (5.1.7.1)$$

and there is *total reflection*. Outside the total-reflection domain, the reflecting power is given by

$$I_h = \left[|\eta| - (\eta^2 - 1)^{1/2} \right]^2. \quad (5.1.7.2)$$

The rocking curve has the well known top-hat shape (Fig. 5.1.7.1). Far from the total-reflection domain, the curve can be

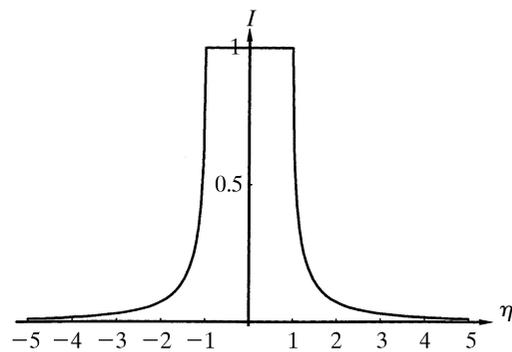


Fig. 5.1.7.1. Theoretical rocking curve in the reflection case for a non-absorbing thick crystal in terms of the deviation parameter.