

## 5.1. DYNAMICAL THEORY OF X-RAY DIFFRACTION

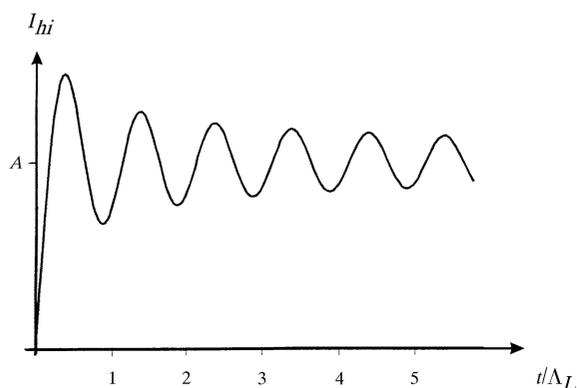


Fig. 5.1.6.7. Variations with crystal thickness of the integrated intensity in the transmission case (no absorption) (arbitrary units). The expression for  $A$  is given in the text.

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

Fig. 5.1.6.7 shows the variations of the integrated intensity with  $t/\Lambda_L$ .

## 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

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

where

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

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  $\xi_j$  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

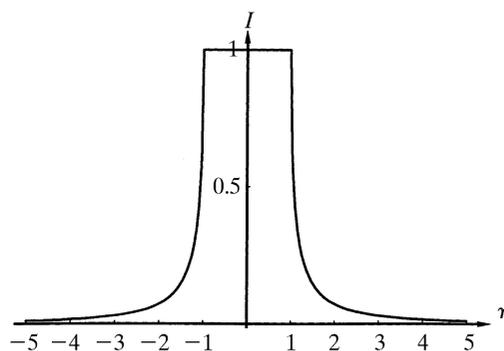


Fig. 5.1.7.1. Theoretical rocking curve in the reflection case for a non-absorbing thick crystal in terms of the deviation parameter.

approximated by the function

$$I_h \approx 1/(4\eta^2).$$

*Width of the total-reflection domain.* The width of the total-reflection domain is equal to  $\Delta\eta = 2$  and its angular width is therefore equal, using (5.1.3.5), to  $2\delta$ , where  $\delta$  is given by (5.1.3.6). It is proportional to the structure factor, the polarization factor  $C$  and the square root of the asymmetry factor  $|\gamma|$ . Using an asymmetric reflection, it is therefore possible to decrease the width at wish. This is used in monochromators to produce a pseudo plane wave [see, for instance, Kikuta & Kohra (1970)]. It is possible to deduce the value of the form factor from very accurate measurements of the rocking curve; see, for instance, Kikuta (1971).

*Integrated intensity.* The integrated intensity is defined by (5.1.6.8):

$$I_{hi} = 8\delta/3. \quad (5.1.7.3)$$

*Penetration depth.* Within the domain of total reflection, there are two wavefields propagating inside the crystal with imaginary wavevectors, one towards the inside of the crystal and the other one in the opposite direction, so that they cancel out and, globally, no energy penetrates the crystal. The absorption coefficient of the waves penetrating the crystal is

$$\mu = -4\pi K_{oi}\gamma_o = 2\pi\gamma_o(1 - \eta^2)^{1/2}/\Lambda_B, \quad (5.1.7.4)$$

where  $\Lambda_B$  is the value taken by  $\Lambda_o$  [equation (5.1.3.8)] in the Bragg case.

The penetration depth is a minimum at the middle of the reflection domain and at this point it is equal to  $\Lambda_B/2\pi$ . This attenuation effect is called *extinction*, and  $\Lambda_B$  is called the *extinction length*. It is a specific property owing to the existence of wavefields. The resulting propagation direction of energy is parallel to the crystal surface, but with a cross section equal to zero: it is an *evanescent wave* [see, for instance, Cowan *et al.* (1986)].

#### 5.1.7.1.2. Absorbing crystals

*Rocking curve.* Since the sign of  $\gamma$  is negative,  $[\eta^2 + S(\gamma h)]^{1/2}$  in (5.1.3.10) has a very large imaginary part when  $|\eta_r| \leq 1$ . It cannot be calculated using the same approximations as in the Laue case. Let us set

$$Z \exp(i\Psi') = \eta \mp (\eta^2 - 1)^{1/2}. \quad (5.1.7.5)$$

The reflecting power is

$$I_h = (F_h/F_{\bar{h}})^{1/2} Z^2, \quad (5.1.7.6)$$

where  $Z = [L - (L^2 - 1)^{1/2}]^{1/2}$ ,  $L = |\eta|^2 + \rho^2$  and  $\rho = |\eta^2 - 1|$  is the modulus of expression (5.1.7.5) where the sign is chosen in such a way that  $Z$  is smaller than 1.

The expression for the reflected intensity in the absorbing Bragg case was first given by Prins (1930). The way of representing it given here was first used by Hirsch & Ramachandran (1950). The properties of the rocking curve have been described by Fingerland (1971).

There is no longer a total-reflection domain and energy penetrates the crystal at all incidence angles, although with a very high absorption coefficient within the domain  $|\eta_r| \leq 1$ . Fig. 5.1.7.2 gives an example of a rocking curve for a thick absorbing crystal. It was first observed by Renninger (1955). The shape is asymmetric and is due to the anomalous-absorption effect: it is lower than normal on the low-angle side, which is associated with wavefields belonging to branch 1 of the dispersion surface, and larger than normal on the high-angle side, which is associated with branch 2 wavefields. The amount of asymmetry depends on the value of the ratio  $A/B$  of the coefficients in the expression for the imaginary part

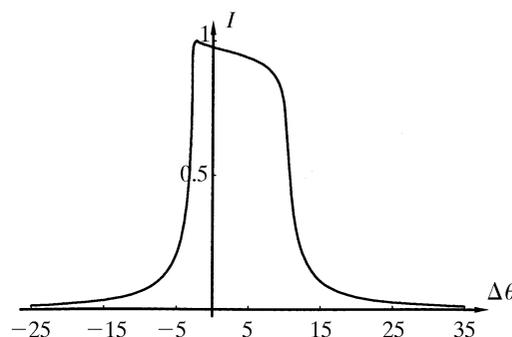


Fig. 5.1.7.2. Theoretical rocking curve in the reflection case for a thick absorbing crystal. The 400 reflection of GaAs using Cu  $K\alpha$  radiation is shown.

of the deviation parameter in (5.1.3.7): the smaller this ratio, the more important the asymmetry.

*Absorption coefficient.* The effective absorption coefficient, taking into account both the Borrmann effect and extinction, is given by (Authier, 1986)

$$\mu = \mu_o + 2(|F_h F_{\bar{h}}|)^{1/2} \frac{R\lambda}{V(|\gamma|)^{1/2}} Z \sin(\beta + \Psi'),$$

where  $\beta$  is defined in equation (5.1.3.7) and  $\Psi'$  in equation (5.1.7.5), and where the sign is chosen in such a way that  $Z$  converges. Fig. 5.1.7.3 shows the variation of the penetration depth  $z_o = \gamma_o/\mu$  with the deviation parameter.

#### 5.1.7.2. Thin crystals

##### 5.1.7.2.1. Non-absorbing crystals

*Boundary conditions.* If the crystal is thin, the wavefield created at the reflecting surface at  $A$  and penetrating inside can reach the back surface at  $B$  (Fig. 5.1.7.4a). The *incident* direction there points towards the *outside* of the crystal, while the *reflected* direction

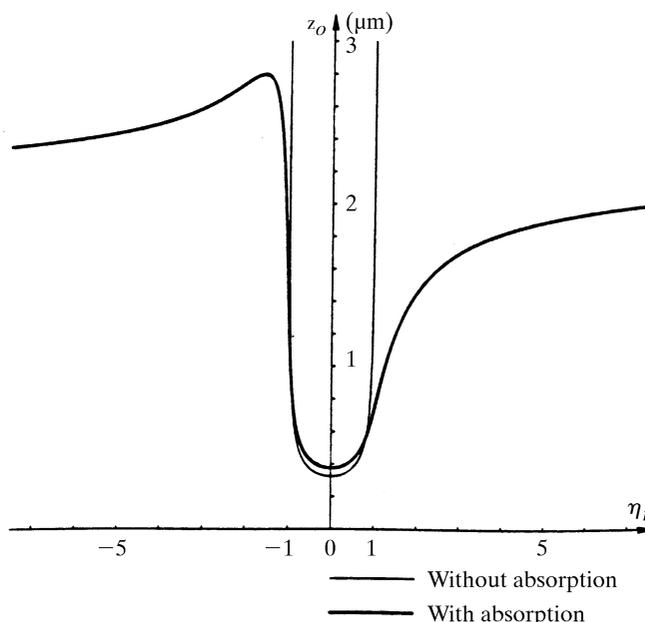


Fig. 5.1.7.3. Bragg case: thick crystals. Variation of the penetration depth with incidence angle (represented here by the dimensionless deviation parameter  $\eta$ ). Thin curve: without absorption; thick curve: with absorption for the 400 reflection of GaAs using Cu  $K\alpha$  radiation.