International Tables for Crystallography (2006). Vol. B, Figure 5.1.7.4, p. 547.

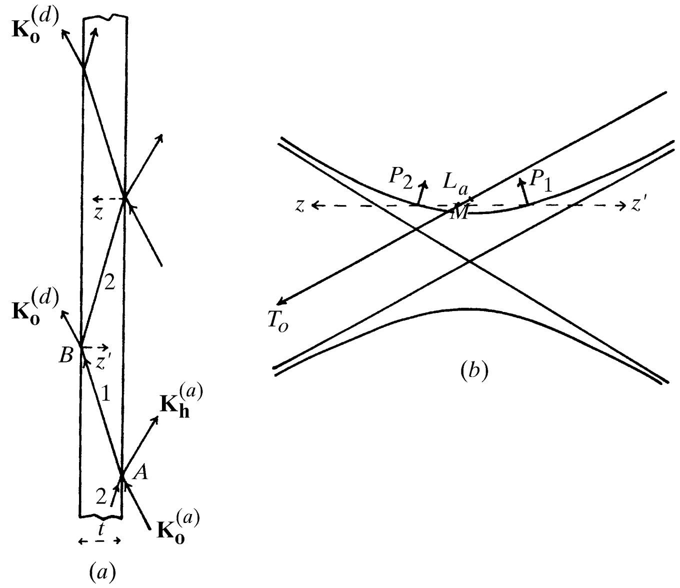

Fig. 5.1.7.4. Bragg case: thin crystals. Two wavefields propagate in the crystal. (*a*) Direct space; (*b*) reciprocal space.

points towards the inside. The wavefield propagating along *AB* will therefore generate at *B*:

(i) *a partially transmitted wave* outside the crystal, $\mathbf{D}_\mathbf{o}^{(d)} \exp(-2\pi i \mathbf{K}_\mathbf{o}^{(d)} \cdot \mathbf{r})$;

(ii) *a partially reflected wavefield* inside the crystal.

The corresponding tiepoints are obtained by applying the usual condition of the continuity of the tangential components of wavevectors (Fig. 5.1.7.4*b*). If the crystal is a plane-parallel slab, these points are *M* and P_2, respectively, and $\mathbf{K}_\mathbf{o}^{(d)} = \mathbf{K}_\mathbf{o}^{(a)}$.

The boundary conditions are then written:

(i) entrance surface:

$$D_{o1} + D_{o2} = D_o^{(a)}, \;\; D_{h1} + D_{h2} = D_h^{(a)};$$

(ii) back surface:

$$D_{o1} \exp(-2\pi i \mathbf{K}_{\mathbf{o}1} \cdot \mathbf{r}) + D_{o2} \exp(-2\pi i \mathbf{K}_{\mathbf{o}2} \cdot \mathbf{r}) = D_o^{(a)} \exp\left(-2\pi i \mathbf{K}_\mathbf{o}^{(d)} \cdot \mathbf{r}\right),$$
$$D_{h1} \exp(-2\pi i \mathbf{K}_{\mathbf{h}1} \cdot \mathbf{r}) + D_{h2} \exp(-2\pi i \mathbf{K}_{\mathbf{h}2} \cdot \mathbf{r}) = 0.$$

Rocking curve. Using (5.1.3.10), it can be shown that the expressions for the intensities reflected at the entrance surface and transmitted at the back surface, I_h and I_o, respectively, are given by different expressions within total reflection and outside it:

(i) $|\eta| < 1$:

$$\left.\begin{aligned} I_h &= |\gamma| \frac{|D_h^{(a)}|^2}{|D_o^{(a)}|^2} = \frac{\cosh^2[\pi(t/\Lambda_B)(1-\eta^2)^{1/2}] - 1}{\cosh^2[\pi(t/\Lambda_B)(1-\eta^2)^{1/2}] - \eta^2} \\ I_o &= \frac{|D_o^{(d)}|^2}{|D_o^{(a)}|^2} = \frac{1-\eta^2}{\cosh^2[\pi(t/\Lambda_B)(1-\eta^2)^{1/2}] - \eta^2}, \end{aligned}\right\} \quad (5.1.7.7a)$$

where Λ_B is the value taken by Λ_o [equation (5.1.3.8)] in the Bragg case.

There is no longer a total-reflection domain but the extinction effect still exists, as is shown by the hyperbolic cosine term. The maximum height of the rocking curve decreases as the thickness of the crystal decreases.

(ii) $|\eta| > 1$:

$$\left.\begin{aligned} I_h &= \frac{1 - \cos^2[\pi(t/\Lambda_B)(\eta^2-1)^{1/2}]}{\eta^2 - \cos^2[\pi(t/\Lambda_B)(\eta^2-1)^{1/2}]}, \\ I_o &= \frac{\eta^2 - 1}{\eta^2 - \cos^2[\pi(t/\Lambda_B)(\eta^2-1)^{1/2}]}. \end{aligned}\right\} \quad (5.1.7.7b)$$

The cosine terms show that the two wavefields propagating within the crystal interfere, giving rise to *Pendellösung* fringes in the rocking curve. These fringes were observed for the first time by Batterman & Hildebrandt (1967, 1968). The angular positions of the minima of the reflected beam are given by

$$\eta = \mp(K^2 \Lambda_B^2 t^{-2} + 1)^{1/2},$$

where *K* is an integer.

Integrated intensity. The integrated intensity is

$$I_{hi} = \pi\delta \tanh[\pi t/\Lambda_B], \quad (5.1.7.8)$$

where *t* is the crystal thickness. When this thickness becomes very large, the integrated intensity tends towards

$$I_{hi} = \pi\delta. \quad (5.1.7.9)$$

This expression differs from (5.1.7.3) by the factor π, which appears here in place of 8/3. von Laue (1960) pointed out that because of the differences between the two expressions for the reflecting power, (5.1.7.2) and (5.1.7.7*b*), perfect agreement could not be expected. Since some absorption is always present, expression (5.1.7.3), which includes the factor 8/3, should be used for very thick crystals. In the presence of absorption, however, expression (5.1.7.8) for the reflected intensity for thin crystals does tend towards that for thick crystals as the crystal thickness increases.

Comparison with geometrical theory. When t/Λ_B is very small (thin crystals or weak reflections), (5.1.7.8) tends towards

$$I_{hi} = R^2 \lambda^2 t |F_h|^2 / (V^2 \gamma_o \sin 2\theta), \quad (5.1.7.10)$$

which is the expression given by geometrical theory. If we call this intensity I_{hi}(geom.), comparison of expressions (5.1.7.8) and (5.1.7.10) shows that the integrated intensity for crystals of intermediate thickness can be written

$$I_{hi} = I_{hi}(\text{geom.}) \frac{\tanh(\pi t/\Lambda_B)}{(\pi t/\Lambda_B)}, \quad (5.1.7.11)$$

which is the expression given by Darwin (1922) for primary extinction.

5.1.7.2.2. *Absorbing crystals*

Reflected intensity. The intensity of the reflected wave for a thin absorbing crystal is

$$\begin{aligned} I_h &= |\gamma| \left| \frac{D_h^{(a)}}{D_o^{(a)}} \right|^2 \\ &= \left| \frac{F_h}{F_{\bar{h}}} \right| \frac{\cosh 2b - \cos 2a}{L \cosh 2b + (L^2-1)^{1/2} \sinh 2b - \cos(2a + 2\Psi')}, \end{aligned} \quad (5.1.7.12)$$

where

$$\left.\begin{aligned} 2a &= [\pi t/\Lambda_B]\rho \cos(\beta + \omega), \\ 2b &= [\pi t/\Lambda_B]\rho \sin(\beta + \omega) \end{aligned}\right\}.$$

references