

5.1. DYNAMICAL THEORY OF X-RAY DIFFRACTION

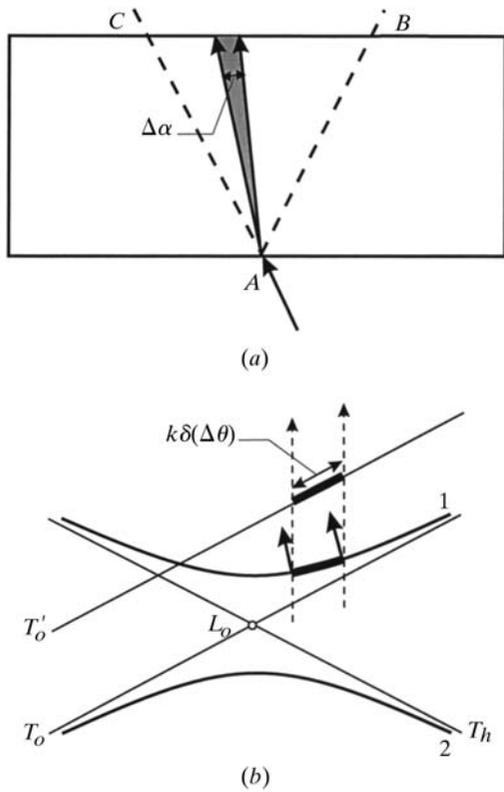


Fig. 5.1.8.2. Packet of wavefields of divergence $\Delta\alpha$ excited in the crystal by an incident wavepacket of angular width $\delta(\Delta\theta)$. (a) Direct space; (b) reciprocal space.

(ii) Large values of $\mu_o t$ (of the order of 6 or more) (Fig. 5.1.8.3b). The predominant factor is now anomalous absorption. The wavefields propagating along the edges of the Borrmann triangle undergo normal absorption, while those propagating parallel to the lattice planes (or nearly parallel) correspond to tie points in the centre of the dispersion surface and undergo anomalously low absorption. The intensity distribution now has a maximum in the centre. For values of μt larger than 10 or so, practically only the wavefields propagating parallel to the lattice planes go through the crystal, which acts as a wave guide: this is the Borrmann effect.

5.1.8.3. Spherical-wave Pendellösung

Fig. 5.1.8.4 shows that along any path Ap inside the Borrmann triangle two wavefields propagate, one with tie point P_1 , on branch 1, the other with the point P_2' , on branch 2. These two points lie on the extremities of a diameter of the dispersion surface. The two wavefields interfere, giving rise to *Pendellösung* fringes, which were first observed by Kato & Lang (1959), and calculated by Kato (1961b). These fringes are of course quite different from the plane-wave *Pendellösung* fringes predicted by Ewald (Section 5.1.6.3) because the tie points of the interfering wavefields are different and their period is also different, but they have in common the fact that they result from interference between wavefields belonging to different branches of the dispersion surface.

Kato has shown that the intensity distribution at any point at the base of the Borrmann triangle is proportional to

$$\left\{ J_o \left[A(x_o x_h)^{1/2} \right] \right\}^2,$$

where $A = 2\pi(\gamma_o \gamma_h)^{1/2} / (\Lambda_L \sin \theta)$ and x_o and x_h are the distances of p from the sides AB and AC of the Borrmann triangle (Fig. 5.1.8.4). The equal-intensity fringes are therefore located along the locus of the points in the triangle for which the product of the distances to the

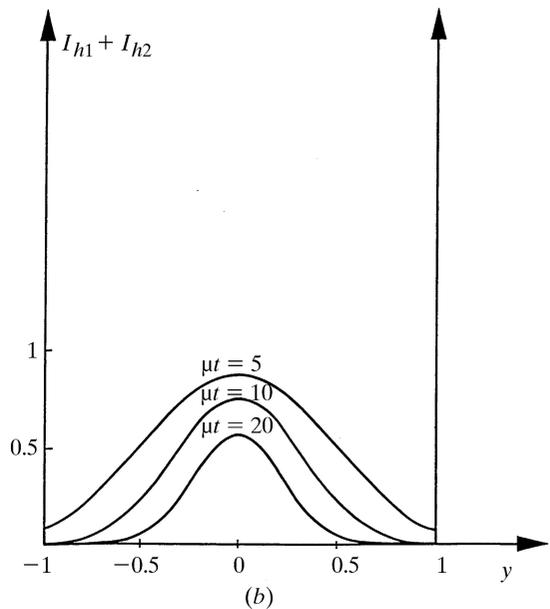
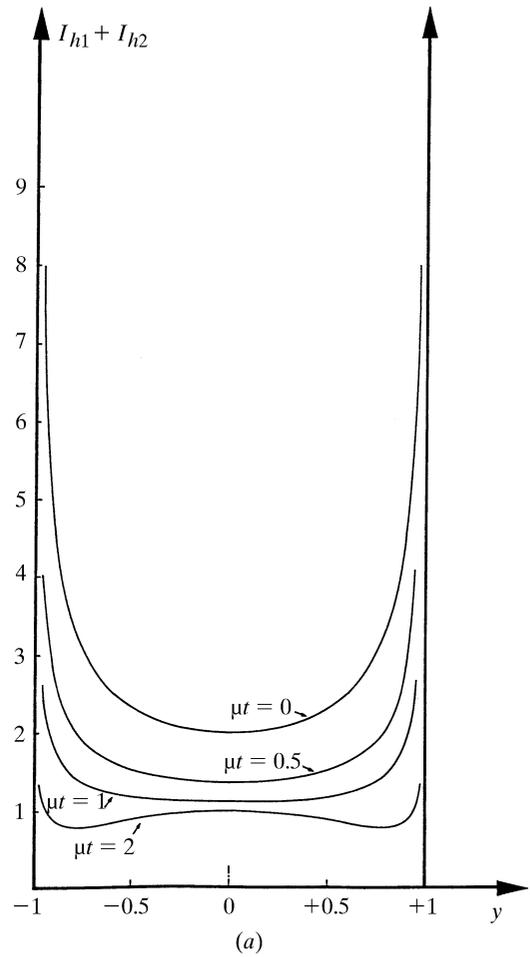


Fig. 5.1.8.3. Intensity distribution along the base of the Borrmann triangle. y is a normalized coordinate along BC . (a) Small values of μt . The interference (spherical-wave *Pendellösung*) between branch 1 and branch 2 is neglected. (b) Large values of μt .

sides is constant, that is hyperbolas having AB and AC as asymptotes (Fig. 5.1.8.4b). These fringes can be observed on a section topograph of a wedge-shaped crystal (Fig. 5.1.8.5). The technique of section topography is described in *IT C*, Section 2.7.2.2. The *Pendellösung* distance Λ_L depends on the polarization

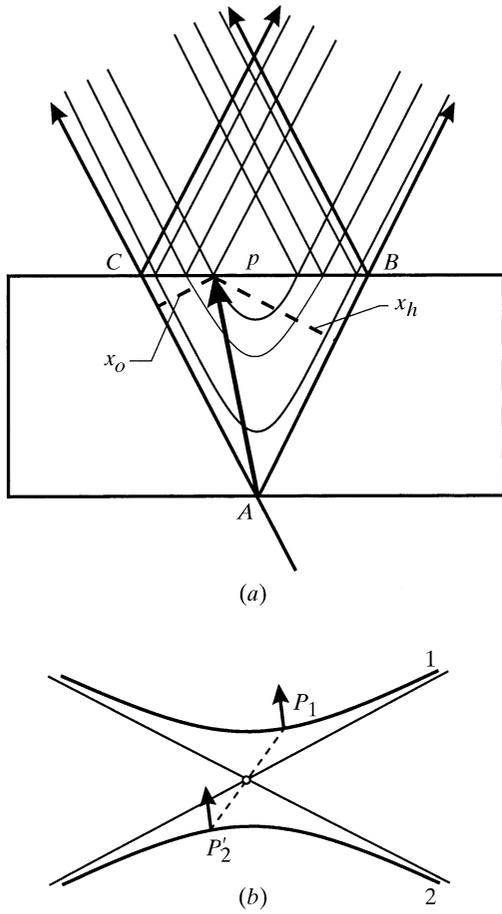


Fig. 5.1.8.4. Interference at the origin of the *Pendellösung* fringes in the case of an incident spherical wave. (a) Direct space; (b) reciprocal space.

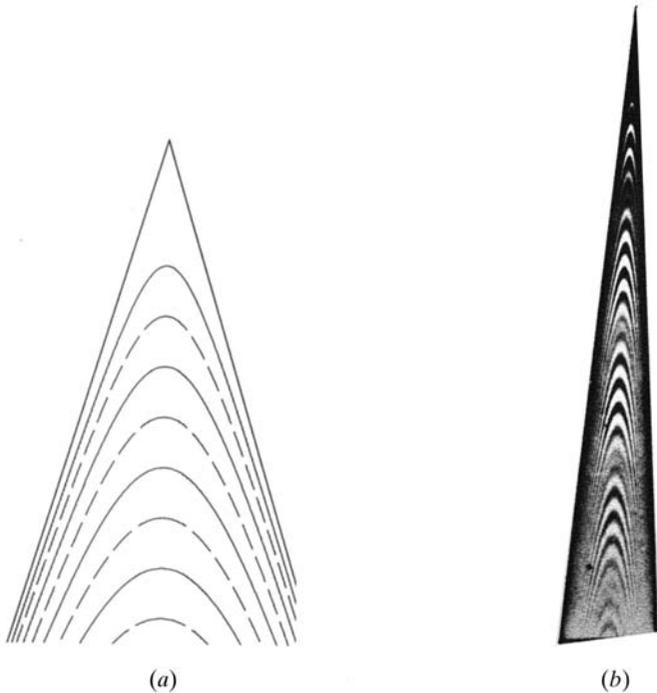


Fig. 5.1.8.5. Spherical-wave *Pendellösung* fringes observed on a wedge-shaped crystal. (a) Computer simulation (solid lines: maxima; dashed lines: minima). (b) X-ray section topograph of a wedge-shaped silicon crystal (444 reflection, Mo $K\alpha$ radiation).

state [see equation (5.1.3.8)]. If the incident wave is unpolarized, one observes the superposition of the *Pendellösung* fringes corresponding to the two states of polarization, parallel and perpendicular to the plane of incidence. This results in a beat effect, which is clearly visible in Fig. 5.1.8.5.

Appendix 5.1.1.

A5.1.1.1. *Dielectric susceptibility – classical derivation*

Under the influence of the incident electromagnetic radiation, the medium becomes polarized. The dielectric susceptibility, which relates this polarization to the electric field, thus characterizes the interaction of the medium and the electromagnetic wave. The classical derivation of the dielectric susceptibility, χ , which is summarized here is only valid for a very high frequency which is also far from an absorption edge. Let us consider an electromagnetic wave,

$$\mathbf{E} = \mathbf{E}_0 \exp 2\pi i(\nu t - \mathbf{k} \cdot \mathbf{r}),$$

incident on a bound electron. The electron behaves as if it were held by a spring with a linear restoring force and is an oscillator with a resonant frequency ν_0 . The equation of its motion is written in the following way:

$$m \, d^2 \mathbf{a} / dt^2 = -4\pi^2 \nu_0 m \mathbf{a} = \mathbf{F},$$

where the driving force \mathbf{F} is due to the electric field of the wave and is equal to $-e\mathbf{E}$. The magnetic interaction is neglected here.

The solution of the equation of motion is

$$\mathbf{a} = -e\mathbf{E} / [4\pi^2 m (\nu_0 - \nu^2)].$$

The resonant frequencies of the electrons in atoms are of the order of the ultraviolet frequencies and are therefore much smaller than X-ray frequencies. They can be neglected and the expression of the amplitude of the electron reduces to

$$\mathbf{a} = e\mathbf{E} / (4\pi^2 \nu^2).$$

The dipolar moment is therefore

$$\mathcal{M} = -e\mathbf{a} = -e^2 \mathbf{E} / (4\pi^2 \nu^2 m).$$

von Laue assumes that the negative charge is distributed continuously all over space and that the charge of a volume element $d\tau$ is $-e\rho \, d\tau$, where ρ is the electronic density. The electric moment of the volume element is

$$d\mathcal{M} = -e^2 \rho \mathbf{E} \, d\tau / (4\pi^2 \nu^2 m).$$

The polarization is equal to the moment per unit volume:

$$\mathbf{P} = d\mathcal{M} / d\tau = -e^2 \rho \mathbf{E} / (4\pi^2 \nu^2 m).$$

It is related to the electric field and electric displacement through

$$\mathbf{D} = \epsilon_0 \mathbf{E} + \mathbf{P} = \epsilon_0 (1 + \chi) \mathbf{E}. \tag{A5.1.1.1}$$

We finally obtain the expression of the dielectric susceptibility,

$$\chi = -e^2 \rho / (4\pi^2 \epsilon_0 \nu^2 m) = -R \lambda^2 \rho / \pi, \tag{A5.1.1.2}$$

where $R = e^2 / (4\pi \epsilon_0 m c^2)$ ($= 2.81794 \times 10^{-15} \text{ m}$) is the classical radius of the electron.

A5.1.1.2. *Maxwell's equations*

The electromagnetic field is represented by two vectors, \mathbf{E} and \mathbf{B} , which are the electric field and the magnetic induction, respectively. To describe the interaction of the field with matter, three other vectors must be taken into account, the electrical current density, \mathbf{j} , the electric displacement, \mathbf{D} , and the magnetic field, \mathbf{H} . The space and time derivatives of these vectors are related in a continuous