

5.1. DYNAMICAL THEORY OF X-RAY DIFFRACTION

increases with increasing wavelength and increasing structure factor. For example, for the 220 reflection of silicon and Cu $K\alpha$ radiation, it is 5.2 seconds.

5.1.3.6. Solution of the dynamical theory

The coordinates of the tie points excited by the incident wave are obtained by looking for the intersection of the dispersion surface, (5.1.2.22), with the normal \mathbf{Mz} to the crystal surface (Figs. 5.1.3.4 and 5.1.3.5). The ratio ξ of the amplitudes of the waves of the corresponding wavefields is related to these coordinates by (5.1.2.24) and is found to be

$$\begin{aligned} \xi_j &= D_{hj}/D_{oj} \\ &= -S(C)S(\gamma_h)[(F_h F_{\bar{h}})^{1/2}/F_{\bar{h}}] \\ &\quad \times \left\{ \eta \pm [\eta^2 + S(\gamma_h)]^{1/2} \right\} / (|\gamma|)^{1/2}, \end{aligned} \quad (5.1.3.10)$$

where the plus sign corresponds to a tie point on branch 1 ($j = 1$) and the minus sign to a tie point on branch 2 ($j = 2$), and $S(\gamma_h)$ is the sign of γ_h (+1 in transmission geometry, -1 in reflection geometry).

5.1.3.7. Geometrical interpretation of the solution in the zero-absorption case

5.1.3.7.1. Transmission geometry

In this case (Fig. 5.1.3.4) $S(\gamma_h)$ is +1 and (5.1.3.10) may be written

$$\xi_j = -S(C)[\eta \pm (\eta^2 + 1)^{1/2}]/\gamma^{1/2}. \quad (5.1.3.11)$$

Let A_1 and A_2 be the intersections of the normal to the crystal surface drawn from the Lorentz point L_o with the two branches of the dispersion surface (Fig. 5.1.3.4). From Sections 5.1.3.3 and 5.1.3.4, they are the tie points excited for $\eta = 0$ and correspond to the middle of the reflection domain. Let us further consider the tangents to the dispersion surface at A_1 and A_2 and let I_{o1} , I_{o2} and I_{h1} , I_{h2} be their intersections with T_o and T_h , respectively. It can be shown that $\overline{I_{o1}I_{h2}}$ and $\overline{I_{o2}I_{h1}}$ intersect the dispersion surface at the tie points excited for $\eta = -1$ and $\eta = +1$, respectively, and that the *Pendellösung* distance $\Lambda_L = 1/A_2A_1$, the width of the rocking curve $2\delta = \overline{I_{o1}I_{o2}}/k$ and the deviation parameter $\eta = \overline{M_oM_h}/A_2A_1$, where M_o and M_h are the intersections of the normal to the crystal surface drawn from the extremity of any incident wavevector \mathbf{OM} with T_o and T_h , respectively.

5.1.3.7.2. Reflection geometry

In this case (Fig. 5.1.3.5) $S(\gamma_h)$ is now -1 and (5.1.3.10) may be written

$$\xi_j = S(C)[\eta \pm (\eta^2 - 1)^{1/2}]/|\gamma|^{1/2}. \quad (5.1.3.12)$$

Now, let I_1 and I_2 be the points of the dispersion surface where the tangent is parallel to the normal to the crystal surface, and further let I_{o1} , I_{h1} , I' and I_{o2} , I_{h2} , I'' be the intersections of these two tangents with T_o , T_h and T'_o , respectively. For an incident wave of wavevector \mathbf{OM} where M lies between I' and I'' , the normal to the crystal surface drawn from M has no real intersection with the dispersion surface and $\overline{I'I''}$ defines the total-reflection domain. The tie points I_1 and I_2 correspond to $\eta = -1$ and $\eta = +1$, respectively, the extinction distance $\Lambda_L = 1/\overline{I_{o1}I_{h1}}$, the width of the total-reflection domain $2\delta = \overline{I_{o1}I_{o2}}/k = \overline{I'I''}/k$ and the deviation parameter $\eta = -\overline{M_oM_h}/\overline{I_{o1}I_{h1}}$, where M_o and M_h are the intersections with T_o and T_h of the normal to the

crystal surface drawn from the extremity of any incident wavevector \mathbf{OM} .

5.1.4. Standing waves

The various waves in a wavefield are coherent and interfere. In the two-beam case, the intensity of the wavefield, using (5.1.2.14) and (5.1.2.24), is

$$\begin{aligned} |D|^2 &= |D_o|^2 \exp(4\pi\mathbf{K}_{oi} \cdot \mathbf{r}) \\ &\quad \times [1 + |\xi|^2 + 2C|\xi| \cos 2\pi(\mathbf{h} \cdot \mathbf{r} + \Psi)], \end{aligned} \quad (5.1.4.1)$$

where Ψ is the phase of ξ ,

$$\xi = |\xi| \exp(i\Psi). \quad (5.1.4.2)$$

Equation (5.1.4.1) shows that the interference between the two waves is the origin of *standing waves*. The corresponding nodes lie on planes such that $\mathbf{h} \cdot \mathbf{r}$ is a constant. These planes are therefore parallel to the diffraction planes and their periodicity is equal to d_{hkl} (defined in the caption for Fig. 5.1.2.1a). Their position within the unit cell is given by the value of the phase Ψ .

In the Laue case, Ψ is equal to $\pi + \varphi_h$ for branch 1 and to φ_h for branch 2, where φ_h is the phase of the structure factor, (5.1.2.6). This means that the *nodes* of standing waves lie on the maxima of the hkl Fourier component of the electron density for branch 1 while the *anti-nodes* lie on the maxima for branch 2.

In the Bragg case, Ψ varies continuously from $\pi + \varphi_h$ to φ_h as the angle of incidence is varied from the low-angle side to the high-angle side of the reflection domain by rocking the crystal. The nodes lie on the maxima of the hkl Fourier components of the electron density on the low-angle side of the rocking curve. As the crystal is rocked, they are progressively shifted by half a lattice spacing until the anti-nodes lie on the maxima of the electron density on the high-angle side of the rocking curve.

Standing waves are the origin of the phenomenon of anomalous absorption, which is one of the specific properties of wavefields (Section 5.1.5). Anomalous scattering is also used for the location of atoms in the unit cell at the vicinity of the crystal surface: when X-rays are absorbed, fluorescent radiation and photoelectrons are emitted. Detection of this emission for a known angular position of the crystal with respect to the rocking curve and therefore for a known value of the phase Ψ enables the emitting atom within the unit cell to be located. The principle of this method is due to Batterman (1964, 1969). For reviews, see Golovchenko *et al.* (1982), Materlik & Zegenhagen (1984), Kovalchuk & Kohn (1986), Bedzyk (1988), Authier (1989), Zegenhagen (1993), Patel (1996), Patel & Fontes (1996), Lagomarsino (1996), Zegenhagen *et al.* (1997), Vartanyants & Zegenhagen (1999) and Vartanyants & Koval'chuk (2001).

5.1.5. Anomalous absorption

It was shown in Section 5.1.2.2 that the wavevectors of a given wavefield all have the same imaginary part (5.1.2.17) and therefore the same absorption coefficient μ (5.1.2.19). Borrmann (1950, 1954) showed that this coefficient is much smaller than the normal one (μ_o) for wavefields whose tie points lie on branch 1 of the dispersion surface and much larger for wavefields whose tie points lie on branch 2. The former case corresponds to the *anomalous transmission effect*, or *Borrmann effect*. As in favourable cases the minimum absorption coefficient may be as low as a few per cent of μ_o , this effect is very important from both a fundamental and a practical point of view.

The physical interpretation of the Borrmann effect is to be found in the standing waves described in Section 5.1.4. When the