*International Tables for Crystallography* (2006). Vol. C, Section 6.4.12, p. 612.



is raised (the polarization index $n$) is 2. In the pure primary-extinction limit, $E_\sigma = 1/(N_c\lambda F\ell)$, while $E_\pi = 1/(N_c\lambda F\ell\cos 2\theta)$. Hence, $n = 1$. In the pure secondary-extinction limit, $E_\sigma = 1/(gQL)$, where $g$ is the mosaic-spread parameter, while $E_\pi = 1/(QgL\cos 2\theta)$. Hence, $n = 0$. In all real cases, $n$ will lie between 0 and 2, and its value will reflect departures from kinematic behaviour.

## 6.4.12. Anisotropy

The parameters describing the microstructure of the crystal are the mosaic-block size and the angle between the mosaic blocks. These are not constrained in any way to be isotropic with respect to the crystal axes. In particular, they are not constrained by symmetry. For example, in a face-centred-cubic crystal under uniaxial stress, slip will occur on one set of {111} planes, leading to a dislocation array of non-cubic symmetry. In principle, anisotropy can be incorporated into the formal theory by allowing $\ell$ and $g$ to depend on the Miller indices of the reflections. This has not been done in this work, but reference should be made to the work of Coppens & Hamilton (1970).

## 6.4.13. Asymptotic behaviour of the integrated intensity

From the definition of the extinction factor, the integrated intensity from a non-absorbing crystal in which the block size is sufficiently small, and the mosaic spread is sufficiently large, will approach the kinematic limit. It is instructive to examine the behaviour in the limit of large block size and low mosaic spread. The volume of the mosaic block is $v$ and the volume of the crystal is $V$. The number of blocks in the crystal is $V/v$ $(= L^3/\ell^3)$. The surface area of the block is $v^{2/3}$ and of the crystal is $V^{2/3}$. The subscripts $L$ and $B$ will again be used for the Laue and the Bragg case, respectively. The kinematic integrated intensity is given by

$$I^{\rm kin} = Q_\theta V = \lambda^3 N_c^2 F^2 V/\sin 2\theta. \qquad (6.4.13.1)$$

6.4.13.1. *Non-absorbing crystal, strong primary extinction*

(*a*) *Laue case*

The limiting value of $E_L$ is $(2/\pi)^{1/2}x^{-1/2}$. Hence,

$$I_L = (4/5)N_c\lambda^2 FVv^{-1/3}/\sin 2\theta. \qquad (6.4.13.2)$$

The dynamical theory has a numerical constant of 1/2 instead of 4/5.

(*b*) *Bragg case*

The limiting value of $E_B$ is $x^{-1/2}$. Hence,

$$I_B = N_c\lambda^2 FVv^{-1/3}/\sin 2\theta. \qquad (6.4.13.3)$$

This is in exact agreement with the dynamical theory (Ewald solution).

6.4.13.2. *Non-absorbing crystal, strong secondary extinction*

For this condition, the limiting values of the integrated intensity are $I_L = (4/5)g^{-1}V^{2/3}$, and $I_B = g^{-1}V^{2/3}$. In this limit, which was also noted by Bacon & Lowde (1948) and by Hamilton (1957), the intensity is proportional only to the mosaic spread and to the surface area of the crystal. No structural information is obtained from the experiment.

6.4.13.3. *The absorbing crystal*

Only the Bragg case for thick crystals will be considered here. The asymptotic values of $A$, $B$, and $C$ are $1/(2\mu L^*)$, $1/(\mu L^*)$, and $2/(\mu L^*)$, respectively, so that

$$BCx = 2N_c^2\lambda^2F^2/\mu^2. \qquad (6.4.13.4)$$

For $BCx$ small, the integrated intensity, $I_B$, is given by

$$I_B = (Q_\theta/2\mu)[1 - (N_cF/)2]V^{2/3}. \qquad (6.4.13.5)$$

For $BCx$ large,

$$I_B = (1/2\sqrt{2})[1 - (\mu/2\lambda N_cF)^2]\lambda^2 N_c FV^{2/3}/\sin 2\theta. \qquad (6.4.13.6)$$

It can be shown that the parameter $g$ (which has no relation to the parameter $g$ used to describe the mosaic-block distribution) used by Zachariasen (1945) in discussing this case is equal to $-\mu/2NCF$. Hence, on his $y$ scale,

$$I_B = (\pi/2\sqrt{2})[1 - g^2]. \qquad (6.4.13.7)$$

The value he obtained is $I_B = 8/3[1 - 2|g|]$, while Sabine & Blair (1992) found $I_B = 8/3[1 - 2.36|g|]$.

## 6.4.14. Relationship with the dynamical theory

Sabine & Blair have shown that the two classical limits for the integrated intensity in the symmetric Bragg case can be obtained from the Hamilton–Darwin equations when the dynamic refractive index of the crystal is explicitly taken into account. Their treatment is based on the following expression for $\sigma(\Delta k)$:

$$\sigma(\Delta k) = \frac{Q_k\mu DT}{\sinh(\mu D)}\left\{\frac{\sin^2(\pi\,T\Delta K) + \sinh^2(\mu D/2)}{(\pi T\Delta K)^2 + (\mu D/2)^2}\right\},$$

where $\Delta K$ refers to the scattering vector within the crystal. Use of the relation $\Delta K \cong \Delta k$ and the replacement of the Fresnellian by a Lorentzian leads to equation (6.4.5.1) with the inclusion of $C$ (6.4.5.2). The relationship between $\Delta K$ and $\Delta k$, which is a function of the dynamic refractive index of the crystal, is derived in the original publication. Insertion of this expression into equations (6.4.4.3) and (6.4.4.4) and integration over $\Delta k$, since the diffracted beam is observed outside the crystal, leads to a dynamic extinction factor, which can be compared with the values determined from the equations given in Section 6.4.5. The integrations cannot be carried out analytically and require numerical calculation in each case.

Olekhnovich & Olekhnovich (1978, 1980) have given limited expressions for primary extinction in the parallelepiped and the cylinder based on the equations of the dynamical theory in the non-absorbing case. Comparisons with the results of the present theory are given by Sabine (1988) and Sabine, Von Dreele & Jørgensen (1988).

## 6.4.15. Definitions

The quantity $F$ used in these equations is the modulus of the structure factor per unit cell. It includes the Debye–Waller factor and the scattering length of each atom. (For X-ray diffraction, the scattering length of the electron is $2.8178 \times 10^{-15}$ m.) $\lambda$ is the wavelength of the incident radiation. $2\theta$ is the angle of scattering. $N_c$ is the number of unit cells per unit volume. The path length of the diffracted beam is $D$, while $T$ is the thickness of the crystal normal to the diffracting plane. In practice, when the orientation of the crystal is unknown, $D$ can be taken equal to $\ell$ or $L$, where these are average dimensions of the mosaic block or crystal.





references