6.2. Trigonometric intensity factors

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6.2.1. Expressions for intensity of diffraction

The expressions for the intensity of diffraction of X-rays contain several trigonometrical factors. The earlier series of *International Tables* (Kasper & Lonsdale, 1959, 1972) gave extensive tables of these functions, but such tables are now unnecessary, as the functions are easily computed. In fact, many crystallographers can ignore the trigonometric factors entirely, as they are built into 'black-box' data-processing programs. The formulae for single-crystal reflections (*b*) and (*c*) of Table 6.2.1.1 in the previous edition (Lipson & Langford, 1998) list only the integrated reflection power ratio (*i.e.* integrated reflection) under the strong absorption case. The revised formulae given here include both the reflection power ratio and the integrated reflection power ratio for a crystal slab of finite thickness with any values of the ratio of the absorption to the diffraction cross sections and under all possible kinds of diffraction geometry.

A conspectus of the expressions for the intensity of diffraction as recorded by various techniques, including the fundamental constants as well as the trigonometric factors, is given in Table 6.2.1.1. Details of the techniques are given elsewhere in this volume (Chapters 2.1–2.3) and in textbooks, such as those of Arndt & Willis (1966) for single-crystal diffractometry and Klug & Alexander (1974) for powder techniques. Notes on individual factors follow.

6.2.2. The polarization factor

X-rays are an electromagnetic radiation, and the amplitude with which they are scattered is proportional to the sine of the angle between the direction of the electric vector of the incident radiation and the direction of scattering. Synchrotron radiation is practically plane-polarized, with the electric vector in the plane of the ring, but the radiation from an ordinary X-ray tube is unpolarized, and it may thus be regarded as consisting of two equal parts, half with the electric vector in the plane of scattering, and half with the electric vector perpendicular to this plane. For the latter, the relevant angle is $\pi/2$, and for the former it is $(\pi/2) - 2\theta$. The intensity is proportional to the square of the amplitude, so that the polarization factor – really the non-polarization factor – is

$$\begin{aligned}&\{\sin^2(\pi/2) + \sin^2[(\pi/2) - 2\theta)]\}/2\\ &\quad = (1 + \cos^2 2\theta)/2. \qquad (6.2.2.1)\end{aligned}$$

If the radiation has been 'monochromatized' by reflection from a crystal, it will be partially polarized, and the two parts of the beam will be of unequal intensity. The intensity of reflection then depends on the angular relations between the original, the reflected, and the scattered beams, but in the commonest arrangements all three are coplanar. The polarization factor then becomes

$$(1 + A\cos^2 2\theta)/(1 + A), \qquad (6.2.2.2)$$

where

$$A = \cos^2 2\theta_M \qquad (6.2.2.3)$$

and θ_M is the Bragg angle of the monochromator crystal. The expression (6.2.2.2) may be substituted for (6.2.2.1) in Table 6.2.1.1 whenever appropriate.

6.2.3. The angular-velocity factor

In experiments where the crystal is rotated or oscillated, reflection of X-rays takes place as a reciprocal-lattice point moves through the surface of the sphere of reflection. The intensity is thus proportional to the time required for the transit of the point through the surface, and so is inversely proportional to the component of the velocity perpendicular to the surface. In most experimental arrangements – the precession camera (Buerger, 1944) is an exception – the crystals move with a constant angular velocity, and the perpendicular component of the velocity varies in an easily calculable way with the 'latitude' of the reciprocal-lattice point referred to the axis of rotation. If the reciprocal-lattice point lies in the equatorial plane and the radiation is monochromatic – the most important case in practice – the angular-velocity factor is

$$\operatorname{cosec} 2\theta. \qquad (6.2.3.1)$$

If the latitude of the reciprocal-lattice point is φ, a somewhat more complex calculation shows that the factor becomes

$$\operatorname{cosec} \theta(\cos^2\varphi - \sin^2\theta)^{1/2}. \qquad (6.2.3.2)$$

For $\varphi = 0$, the expression (6.2.3.2) reduces to (6.2.3.1). In some texts, φ is used for the co-latitude; this and various trigonometric identities can give superficially very different appearances to (6.2.3.2).

6.2.4. The Lorentz factor

There has been some argument over the meaning to be attached to the term *Lorentz factor*, probably because Lorentz did not publish his results in the ordinary way; they appear in a note added in proof to a paper on temperature effects by Debye (1914). Ordinarily, *Lorentz factor* is used for the trigonometric part of the angular-velocity factor, or its equivalent, if the sample is stationary. (See below).

6.2.5. Special factors in the powder method

In the powder method, all rays diffracted through an angle 2θ lie on the surface of a cone, and in the absence of preferred orientation the diffracted intensity is uniformly distributed over the circumference of the cone. The amount effective in blackening film, or intercepted by the receiving slit of a diffractometer, is thus inversely proportional to the circumference of the cone, and directly proportional to the fraction of the crystallites in a position to reflect. When allowance is made for these geometrical factors, it is found that for the Debye–Scherrer and diffractometer arrangements the intensity is proportional to

$$p'' \operatorname{cosec} \theta, \qquad (6.2.5.1)$$

where p'' is the multiplicity factor (the number of permutations of *hkl* leading to the same value of θ). For the flat-plate front-reflection arrangement, the variation becomes

$$p'' \cos 2\theta \operatorname{cosec} \theta. \qquad (6.2.5.2)$$

Combining the polarization, angular-velocity, and special factors gives a trigonometric variation of

$$p''(1 + \cos^2 2\theta)\sec\theta\operatorname{cosec}^2\theta \qquad (6.2.5.3)$$

references