Table 6.2.1.1. *Summary of formulae for integrated powers of reflection (cont.)*

Symbols	
c	Speed of light
λ	Wavelength of radiation
μ	Linear absorption coefficient for X-rays or total attenuation coefficient for neutrons
2θ	Angle between incident and diffracted beams
φ	In (*b*) and (*c*), as defined; in (*h*), latitude of reciprocal-lattice point relative to axis of rotation
V	Volume of crystal, or of irradiated part of powder sample
N	Number of unit cells per unit volume
ξ	In (*b*) and (*c*), as defined; in (*h*), radial coordinate *xi* used in interpreting Weissenberg photographs
I_0	Energy of radiation falling normally on unit area per second
hkl	Indices of reflection
F	Structure factor of *hkl* reflection
$W(\Delta\theta_0)$	Distribution function of the mosaic blocks at angular deviation $\Delta\theta_0$ from the average reflecting plane
σ	Diffraction cross section per unit volume
σ_0	Diffraction cross section per unit volume at $\Delta\theta_0 = 0$
b	Asymmetry parameter
τ	Reduced thickness of the crystal slab
P_H/P_0	Reflection power ratio, *i.e.* the ratio of diffracted power to the incident power
ρ	Integrated reflection power ratio from a crystal element
ρ'	Integrated reflection power ratio, angular integration of reflection power ratio
p'	Multiplicity factor for single-crystal methods
p''	Multiplicity factor for powder methods

for the Debye–Scherrer and diffractometer arrangements, and

$$p''(1+\cos^2 2\theta)\tan 2\theta \operatorname{cosec}\theta \qquad (6.2.5.4)$$

for the flat-plate front-reflection arrangement.

Nowadays, angle-dispersive experiments are normally carried out by stepping the sample and detector in small angular increments, both being stationary while the intensity at each step is recorded. The Lorentz factor for a random powder sample is then of the form $p''(\cos\theta\sin^2\theta)^{-1}$. The factor $\cos\theta$ arises from the fact that spherical shells of diffracted intensity in reciprocal space intersect the Ewald sphere at an angle that depends on θ, and the surface area of the shells increases as d^{*2}, which is emobodied in the factor $\sin^2\theta$. It turns out that this factor is equivalent to a combination of the polarization factor (6.2.2.1), the angular-velocity factor (6.2.3.1) and (6.2.5.1), and the form of (6.2.5.3) is thus unchanged.

6.2.6. Some remarks about the integrated reflection power ratio formulae for single-crystal slabs

The transfer equations for intensity may be rewritten in the form of one-dimensional power transfer equations (Hu & Fang, 1993). The P_H/P_0 in (*b*) and (*c*) for a mosaic crystal slab under symmetrical and unsymmetrical Bragg and Laue geometries are the general solutions of power transfer equations employing three dimensionless parameters b, ξ and τ. For a crystal slab with a rectangular mosaic distribution, considering multiple reflection, the integrated reflection power ratio, ρ', can be obtained by substituting σ_0 for σ in the formulae for P_H/P_0 and multiplying the result by the mosaic width. However, for crystals with other kinds of mosaic distribution, the corresponding ρ' can be obtained only by integrating the expression for $P_H(\Delta\theta_0)/P_0$ over the whole range of $\Delta\theta_0$. Formulae (1)–(3) listed in Table 6.3.3.1, *i.e.* the transmission coefficient A multiplied by Q, QA, are identical to those of (*b*) and (*c*) for the case of $\mu/\sigma_0 >> 1$, which is the integrated reflection power ratio for a crystal slab based on the kinematic approximation without consideration of multiple reflection.

The secondary extinction factor for X-ray or neutron diffraction in a mosaic crystal slab can be obtained as $\rho'/(QA)$, in which the integrated reflection power ratio with consideration of multiple reflections can be obtained as described above.

Both the transmission power ratio P_T/P_0 and the absorption power ratio P_A/P_0 can also be obtained by solving the power transfer equations. For details, see Hu (1997*a*,*b*), Werner & Arrott (1965) and Werner, Arrott, King & Kendrick (1966).

6.2.7. Other factors

The various expressions in Table 6.2.1.1 contain $|F|^2$, the square of the modulus of the structure factor. The relation of F to the atomic scattering factors, the atomic positional coordinates, and the temperature is treated in Chapter 6.1.

For the factors relevant for the precession method (Buerger, 1944), see Waser (1951*a*,*b*), Burbank (1952), and Grenville-Wells & Abrahams (1952). For the de Jong–Bouman method, see Bouman & de Jong (1938) and Buerger (1940). For the retigraph, see Mackay (1960).

references