$$\rho = \frac{\Theta}{b(D\ell)^{1/2}}, \qquad (6.4.3.1)$$

where ρ is the dislocation density, Θ is the total mosaic spread in radians, b is the Burgers vector of the dislocations, ℓ is the block size and D is the size of the irradiated region.

6.4.4. Radiation flow

The radiation flow is governed by the Hamilton–Darwin (H–D) equations (Darwin, 1922; Hamilton, 1957). These equations are

$$\frac{\partial P_i}{\partial t_i} = \tau P_i + \sigma P_f, \qquad (6.4.4.1)$$

$$\frac{\partial P_f}{\partial t_f} = \tau P_f + \sigma P_i. \qquad (6.4.4.2)$$

Here, P_i is the radiation current density ($m^{-2}\,s^{-1}$) in the incident (i = initial) beam, P_f is the current density in the diffracted (f = final) beam. The distances t_i and t_f are measured along the incident and diffracted beams, respectively. The coupling constant σ is the cross section per unit volume for scattering into a single Bragg reflection, while τ, which is always negative, is the cross section per unit volume for removal of radiation from the beams by any process. In what follows, it will be assumed that absorption is the only significant process, and τ is given by $\tau = -(\sigma + \mu)$, where μ is the linear absorption coefficient (absorption cross section per unit volume). This assumption may not be true for neutron diffraction, in which incoherent scattering may have a significant role in removing radiation. In those cases, τ should include the incoherent scattering cross section per unit volume.

The H–D equations have analytical solutions in the Laue case ($2\theta = 0$) and the Bragg case ($2\theta = \pi$). The solutions at the exit surface are, respectively,

$$P_f = \frac{P_i^0}{2}\exp(-\mu D)[1 - \exp(-2\sigma D)], \qquad (6.4.4.3)$$

and

$$P_f = \frac{P_i^0 \sigma \sinh(aD)}{a\cosh(aD) - \tau\sinh(aD)}, \qquad (6.4.4.4)$$

with $a^2 = \tau^2 - \sigma^2$. The path length of the diffracted beam through the crystal is D. The current density at the entrance surface is P_i^0.

To find formulae for the integrated intensity, it is necessary to express σ in terms of crystallographic quantities.

6.4.5. Primary extinction

Zachariasen (1967) introduced the concept of using the kinematic result in the small-crystal limit for σ, while Sabine (1985, 1988) showed that only the Lorentzian or Fresnellian forms of the small crystal intensity distribution are appropriate for calculations of the energy flow in the case of primary extinction. Thus,

$$\sigma(\Delta k) = \frac{Q_k T}{1 + (\pi T \Delta k)^2}, \qquad (6.4.5.1)$$

where $Q_k V$ is the kinematic integrated intensity on the k scale ($k = 2\sin\theta/\lambda$), $Q_k = (N_c \lambda F)^2/\sin\theta$, and T is the volume average of the thickness of the crystal normal to the diffracting plane (Wilson, 1949). To include absorption effects, which modify the diffraction profile of the small crystal, it is necessary to replace T by TC, where

$$C = \frac{\tanh(\mu D/2)}{(\mu D/2)}. \qquad (6.4.5.2)$$

To determine the extinction factor, E, the explicit expression for $\sigma(\Delta k)$ [equation (6.4.5.1)] is inserted into equations (6.4.4.3) and (6.4.4.4), and integration is carried out over Δk. The limits of integration are $+\infty$ and $-\infty$. The notation E_L and E_B is used for the extinction factors at $2\theta = 0$ and $2\theta = \pi$ rad, respectively.

After integration and division by $I^{\rm kin}$, it is found that

$$E_L = \exp(-y)\{[1 - (x/2) + (x^2/4) - (5x^3/48) + (7x^4/192)]\}, \quad x \le 1, \qquad (6.4.5.3)$$

$$E_L = \exp(-y)[2/(\pi x)]^{1/2}\{1 - [1/(8x)] - [3/(128x^2)] - [15/(1024x^3)]\}, \quad x > 1, \qquad (6.4.5.4)$$

$$E_B = A/(1 + Bx)^{1/2}, \qquad (6.4.5.5)$$

$$A = \exp(-y)\sinh y/y, \qquad (6.4.5.6)$$

and

$$B = (1/y) - \exp(-y)/\sinh y = A\frac{{\rm d}(A^{-1})}{{\rm d}y}. \qquad (6.4.5.7)$$

In these equations, $x = Q_k TCD$ and $y = \mu D$.

6.4.6. The finite crystal

Exact application of the formulae above requires a knowledge of the shape of the crystal or mosaic block and the angular relation between the reflecting plane and the crystal surface. These are not usually known, but it can be assumed that the average block or crystal at each value of the scattering angle (2θ) has sides of equal length parallel to the incident- and diffracted-beam directions. For this crystal,

$$T = D\sin\theta, \;\; D = \langle L\rangle, \qquad (6.4.6.1)$$

and

$$x = N_c{}^2\lambda^2F^2\langle L\rangle^2\tanh(\mu L^*/2)/(\mu L^*/2). \qquad (6.4.6.2)$$

The quantity L^* is set equal to ℓ for the mosaic block and to L for the crystal.

6.4.7. Angular variation of *E*

Werner (1974) has given exact solutions to the transport equations in terms of tabulated functions. However, for the simple crystal described above, a sufficiently accurate expression is

$$E(2\theta) = E_L\cos^2\theta + E_B\sin^2\theta. \qquad (6.4.7.1)$$

6.4.8. The value of *x*

For the single mosaic block, application of the relationship $T = D\sin\theta$ leads to

$$x = (N_c\lambda F\ell)^2, \qquad (6.4.8.1)$$

where ℓ is the average path length through the block. In the correlated block model, x is also a function of the tilts between blocks and the size of the crystal.

It will be assumed for the discussion that follows in this section that the mosaic blocks are cubes of side ℓ, and the distribution of tilts will be assumed to be isotropic and Gaussian, given by