

4. DIFFUSE SCATTERING AND RELATED TOPICS

lattice sites, and the lateral and axial lattice disorder weights are given by

$$w_{\text{lat}}(R, r) = \exp(-4\pi^2 R^2 \sigma_{\text{lat}}^2 [1 - \rho_{\text{lat}}(r)]) \quad (4.5.2.42)$$

and

$$w_{\text{axial}}(Z, r) = \exp(-4\pi^2 Z^2 \sigma_{\text{axial}}^2 [1 - \rho_{\text{axial}}(r)]). \quad (4.5.2.43)$$

Equation (4.5.2.41) is an expression for the continuous intensity distribution along the layer lines and does not separate into Bragg and continuous components as in the case of uncorrelated disorder. However, calculations using these expressions show that the continuous intensity is sharply peaked around the projected reciprocal-lattice points at low resolution, the peaks broadening with increasing resolution until they have the character of continuous diffraction at high resolution (Stroud & Millane, 1996a). This is consistent with the character of diffraction patterns from some disordered polycrystalline fibres. A detailed study of the effects of correlated disorder on fibre diffraction patterns, and analysis of such disorder, can be found in Stroud & Millane (1996a) and Stroud & Millane (1996b).

4.5.2.5. Processing diffraction data

Since the diffraction pattern from a fibre is two-dimensional, it can be collected with a single exposure of a stationary specimen. Diffraction data are collected either on film, which is subsequently scanned by a two-dimensional microdensitometer to obtain a digitized representation of the diffracted intensity, or using an electronic area detector (imaging plate, CCD camera, wire detector *etc.*) (Fraser *et al.*, 1976; Namba, Yamashita & Vonderviszt, 1989; Lorenz & Holmes, 1993). We assume here that the diffraction pattern is recorded on a flat film (or detector) that is normal to the incident X-ray beam, although other film geometries are easily accommodated (Fraser *et al.*, 1976). The fibre specimen is usually oriented with its axis normal to the incident X-ray beam, although, as is described below, it is sometimes tilted by a small angle to the normal in order to better access reciprocal space close to the meridian. The diffraction and camera geometry are shown in Fig. 4.5.2.1. Referring to this figure, P and S denote the intersections of the diffracted beam with the sphere of reflection and the film, respectively. The fibre, and therefore reciprocal space, is tilted by an angle β to the normal to the incident beam. The angles μ and χ define the direction of the diffracted beam and θ is the Bragg angle. Cartesian and polar coordinates on the film are denoted by (u, v) and (r, φ) , respectively, and D denotes the film-to-specimen distance.

Inspection of Fig. 4.5.2.1 shows that the cylindrical (R, ψ, Z) and spherical (ρ, ψ, σ) polar coordinates in reciprocal space are related to μ and χ by

$$\rho = (1/\lambda)[2(1 - \cos \mu - \cos \chi)]^{1/2}, \quad (4.5.2.44)$$

$$Z = (1/\lambda)[\sin \beta(1 - \cos \mu \cos \chi) + \cos \beta \sin \chi]^{1/2}, \quad (4.5.2.45)$$

$$R = (\rho^2 - Z^2)^{1/2}, \quad (4.5.2.46)$$

$$\sin \psi = \frac{\sin \mu \cos \chi}{R\lambda} \quad (4.5.2.47)$$

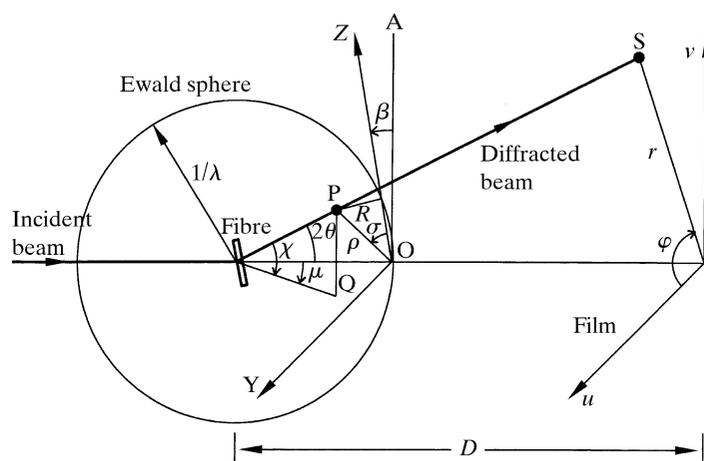


Fig. 4.5.2.1. Fibre diffraction geometry (see text). O is the origin of reciprocal space and \mathbf{OA} is normal to the incident X-ray beam. Reciprocal space is rotated about \mathbf{OY} so that the Z axis is inclined at an angle β to \mathbf{OA} . Q is the projection of P onto the plane containing the incident beam and \mathbf{OY} .

and

$$\tan \sigma = R/Z. \quad (4.5.2.48)$$

The coordinates on the film are related to μ and χ by

$$u = D \tan \mu \quad (4.5.2.49)$$

and

$$v = D \cos \mu \tan \chi, \quad (4.5.2.50)$$

and we also have that

$$r = D \tan 2\theta. \quad (4.5.2.51)$$

Use of the above equations allows the reciprocal-space coordinates to be calculated from film-space coordinates, and *vice versa*. The film coordinates (u, v) represent a relatively undistorted map of reciprocal space (R, Z) , except near the v (vertical) axis of the diffraction pattern. The meridian of reciprocal space does not map onto the film. Inspection of Fig. 4.5.2.1 shows that the only point on the meridian that does appear on the film is at $Z = \lambda^{-1} \sin \beta$. The region *close* to the meridian that appears on the film can therefore be manipulated by adjusting the fibre tilt.

The film-to-specimen distance can be determined by including with the specimen a crystalline power that gives a diffraction ring of known spacing and adjusting the film-to-specimen distance so that the calculated and observed rings coincide. A nonzero fibre tilt leads to differences between the upper and lower halves of the diffraction pattern, and these differences can be used to determine the tilt. This can be done by either calculating the ρ and χ values for several sets of the same reflection above and below the equator and using the relationship

$$\tan \beta = \frac{\sin \chi_U + \sin \chi_L}{\lambda^2 \rho^2}, \quad (4.5.2.52)$$

where χ_U and χ_L refer to the upper and lower ($\chi < 0$) reflections (Millane & Arnott, 1986; Lorenz & Holmes, 1993), or by finding the tilt that minimizes the differences between optical densities at the same reciprocal-space coordinates above and below the