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atom and $\rho = (R^2 + l^2/Z^2)^{1/2}$ is the spherical radius in reciprocal space. Equations (4.5.2.12) and (4.5.2.13) allow the complex diffracted amplitudes for a helical molecule to be calculated from the atomic coordinates, and are analogous to expressions for the structure factors in conventional crystallography.

The significance of the selection rule is now more apparent. On a particular layer plane l , not all Fourier–Bessel structure factors $G_n(R)$ contribute; only those whose Bessel order n satisfies the selection rule for that value of l contribute. Since any molecule has a maximum radius, denoted here by r_{\max} , and since $J_n(x)$ is small for $x < |n| - 2$ and diffraction data are measured out to only a finite value of R , reference to equation (4.5.2.10) [or equation (4.5.2.13)] shows that there is a maximum Bessel order that contributes significant value to equation (4.5.2.12) (Crowther *et al.*, 1970; Makowski, 1982), so that the infinite sum over n in equation (4.5.2.12) can be replaced by a finite sum. On each layer plane there is also a minimum value of $|n|$, denoted by n_{\min} , that satisfies the helix selection rule, so that the region $R < R_{\min}$ is devoid of diffracted amplitude where

$$R_{\min} = \frac{n_{\min} - 2}{2\pi r_{\max}}. \quad (4.5.2.14)$$

The selection rule therefore results in a region around the Z axis of reciprocal space that is devoid of diffraction, the shape of the region depending on the helix symmetry.

4.5.2.3.3. Approximate helix symmetry

In some cases the nature of the subunits and their interactions results in a structure that is not exactly periodic. Consider a helical structure with $u + x$ subunits in v turns, where x is a small ($x \ll 1$) real number; *i.e.* the structure has approximate, but not exact, u_v helix symmetry. Since the molecule has an *approximate* repeat distance c , only those layer planes close to those at $Z = l/c$ show significant diffraction. Denoting by Z_{mn} the Z coordinate of the n th Bessel order and its associated value of m , and using the selection rule shows that

$$Z_{mn} = [(um + vn)/c] + (mx/c) = (l/c) + (mx/c), \quad (4.5.2.15)$$

so that the positions of the Bessel orders are shifted by mx/c from their positions if the helix symmetry is exactly u_v . At moderate resolution m is small so the shift is small. Hence Bessel orders that would have been coincident on a particular layer plane are now separated in reciprocal space. This is referred to as *layer-plane splitting* and was first observed in fibre diffraction patterns from tobacco mosaic virus (TMV) (Franklin & Klug, 1955). Splitting can be used to advantage in structure determination (Section 4.5.2.6.6).

As an example, TMV has approximately 49_3 helix symmetry with a c repeat of 69 Å. However, close inspection of diffraction patterns from TMV shows that there are actually about 49.02 subunits in three turns (Stubbs & Makowski, 1982). The virus is therefore more accurately described as a 2451_{150} helix with a c repeat of 3450 Å. The layer lines corresponding to this larger repeat distance are not observed, but the effects of layer-plane splitting are detectable (Stubbs & Makowski, 1982).

4.5.2.4. Diffraction by fibres

The kind of diffraction pattern obtained from a fibre specimen made up of helical molecules depends on the kind of specimen as described in Section 4.5.2.2. This section is divided into four parts. The first two describe diffraction patterns obtained from noncrystalline and polycrystalline fibres (which are the most common kinds used for structural analysis), and the last two describe diffraction by partially crystalline fibres.

4.5.2.4.1. Noncrystalline fibres

A noncrystalline fibre is made up of a collection of helical molecules that are oriented parallel to each other, but are otherwise randomly positioned and rotated relative to each other. The recorded intensity, $I_l(R)$, is therefore that diffracted by a single molecule cylindrically averaged about the Z axis in reciprocal space *i.e.*

$$I_l(R) = (1/2\pi) \int_0^{2\pi} |F_l(R, \psi)|^2 d\psi; \quad (4.5.2.16)$$

using equation (4.5.2.12) shows that

$$I_l(R) = \sum_n |G_n(R)|^2, \quad (4.5.2.17)$$

where, as usual, the sum is over the values of n that satisfy the helix selection rule. On the diffraction pattern, reciprocal space (R, ψ, Z) collapses to the two dimensions (R, Z) . The R axis is called the *equator* and the Z axis the *meridian*. The layer planes collapse to *layer lines*, at $Z = l/c$, which are indexed by l . Equation (4.5.2.17) gives a rather simple relationship between the recorded intensity and the Fourier–Bessel structure factors.

Coherence length and disorientation, as described in Section 4.5.2.2, also affect the form of the diffraction pattern. These effects are described here, although they also apply to other than noncrystalline fibres. A finite coherence length leads to smearing of the layer lines along the Z direction. If the average coherence length of the molecules is l_c , the intensity distribution $I_l(R, Z)$ about the l th layer line can be approximated by

$$I_l(R, Z) = I_l(R) \exp(-\pi l_c^2 [Z - (l/c)]^2). \quad (4.5.2.18)$$

It is convenient to express the effects of disorientation on the intensity distribution of a fibre diffraction pattern by writing the latter as a function of the polar coordinates (ρ, σ) (where σ is the angle with the Z axis) in (R, Z) space. Assuming a Gaussian orientation density function [equation (4.5.2.1)], if α_0 is small and the effects of disorientation dominate over those of coherence length (which is usually the case except close to the meridian), then the distribution of intensity about one layer line can be approximated by (Holmes & Barrington Leigh, 1974; Stubbs, 1974)

$$I(\rho, \sigma) \simeq \frac{I_l(R)}{2\pi\alpha_0 l_c \rho} \exp\left[-\frac{(\sigma - \sigma_l)^2}{2\beta^2}\right], \quad (4.5.2.19)$$

where (Millane & Arnott, 1986; Millane, 1989c)

$$\beta^2 = \alpha_0^2 + (1/2\pi l_c^2 \rho^2 \sin^2 \sigma_l) \quad (4.5.2.20)$$

and σ_l is the polar angle at the centre of the layer line, *i.e.* $R = \rho \sin \sigma_l$. The effect of disorientation, therefore, is to smear each layer line about the origin of reciprocal space.

4.5.2.4.2. Polycrystalline fibres

A polycrystalline fibre is made up of crystallites that are oriented parallel to each other, but are randomly positioned and randomly rotated about their molecular axes. The recorded diffraction pattern is the intensity diffracted by a single crystallite, cylindrically averaged about the Z axis. On a fibre diffraction pattern, therefore, the Bragg reflections are cylindrically projected onto the (R, Z) plane and their positions are described

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by the cylindrically projected reciprocal lattice (Finkenstadt & Millane, 1998).

The molecules are periodic and are therefore usually aligned with one of the unit-cell vectors. Since the z axis is defined as the fibre axis, it is usual in fibre diffraction to take the \mathbf{c} lattice vector as the unique axis and as the lattice vector parallel to the molecular axes. It is almost always the case that the fibre is rotationally disordered about the molecular axes, *i.e.* about \mathbf{c} . Consider first the case of a monoclinic unit cell ($\alpha = \beta = 90^\circ$) so that the reciprocal lattice is cylindrically projected about \mathbf{c}^* . The cylindrical coordinates of the projected reciprocal-lattice points are then given by

$$R_{hkl}^2 = h^2 a^{*2} + k^2 b^{*2} + 2hka^*b^* \cos \gamma^* \quad (4.5.2.21)$$

and

$$Z_{hkl} = lc^*, \quad (4.5.2.22)$$

so that R depends only on h and k , and Z depends only on l . Reflections with fixed h and k lie on straight *row lines*. Certain sets of distinct reciprocal-lattice points will have the same value of R_{hkl} and therefore superimpose in cylindrical projection. For example, for an orthorhombic system ($\gamma = 90^\circ$) the reciprocal-lattice points (hkl) , $(\bar{h}kl)$, $(h\bar{k}l)$ and $(\bar{h}\bar{k}l)$ superimpose. Furthermore, the crystallites in a fibre specimen are usually oriented randomly up and down so that the reciprocal-lattice points (hkl) and $(\bar{h}\bar{k}l)$ superimpose, so that in the orthorhombic case eight reciprocal-lattice points superimpose. Also, as described below, reciprocal-lattice points that have similar values of R can effectively superimpose.

If the unit cell is either triclinic, or is monoclinic with $\alpha \neq 90^\circ$ or $\beta \neq 90^\circ$, then \mathbf{c}^* is inclined to \mathbf{c} and the Z axis, and the reciprocal lattice is not cylindrically projected about \mathbf{c}^* . Equation (4.5.2.22) for Z_{hkl} still applies, but the cylindrical radius is given by

$$R_{hkl}^2 = h^2 a^{*2} + k^2 b^{*2} + l^2 [c^{*2} - (1/c^2)] + 2hka^*b^* \cos \gamma^* + 2hla^*c^* \cos \beta^* + 2klb^*c^* \cos \alpha^* \quad (4.5.2.23)$$

and the row lines are curved (Finkenstadt & Millane, 1998).

The most complicated situation arises if the crystallites are rotationally disordered about an axis that is inclined to \mathbf{c} . Reciprocal space is then rotated about an axis that is inclined to the normal to the a^*b^* plane, R_{hkl} and Z_{hkl} are both functions of h , k and l , equation (4.5.2.23) does not apply, and reciprocal-lattice points for fixed l do not lie on layer lines of constant Z . Although this situation is rather unusual, it does occur (Daubeny *et al.*, 1954), and is described in detail by Finkenstadt & Millane (1998).

The observed fibre diffraction pattern consists of reflections at the projected reciprocal-lattice points whose intensities are equal to the sums of the intensities of the contributing structure factors. The observed intensity, denoted by $I_l(R_{hk})$, at a projected reciprocal-lattice point on the l th layer line and with $R = R_{hk}$ is therefore given by (assuming, for simplicity, a monoclinic system)

$$I_l(R_{hk}) = \sum_{h', k' \in \mathcal{S}(h, k)} |F_{h'k'l}|^2, \quad (4.5.2.24)$$

where $\mathcal{S}(h, k)$ denotes the set of indices (h', k') such that $R_{h'k'} = R_{hk}$. The number of independent reflections contributing in equation (4.5.2.24) depends on the space-group symmetry of the crystallites, because of either systematic absences or structure factors whose values are related.

The effect of a finite crystallite size is to smear what would otherwise be infinitely sharp reflections into broadened reflections of a finite size. If the average crystallite dimensions normal and parallel to the z axis are l_{lat} (*i.e.* in the 'lateral' direction) and l_{axial} (*i.e.* in the 'axial' direction), respectively, the profile of the reflection centred at $(R_{hk}, Z = l/c)$ can be written as (Fraser *et al.*, 1984; Millane & Arnott, 1986; Millane, 1989c)

$$I(R, Z) = I_l(R_{hk})S(R - R_{hk}, Z - l/c), \quad (4.5.2.25)$$

where the profile function $S(R, Z)$ can be approximated by

$$S(R, Z) = \exp[-\pi(l_{\text{lat}}^2 R^2 + l_{\text{axial}}^2 Z^2)]. \quad (4.5.2.26)$$

The effect of crystallite disorientation is to smear the reflections given by equation (4.5.2.26) about the origin of the projected reciprocal space. If the effects of disorientation dominate over those of crystallite size, then the profile of a reflection can be approximated by (Fraser *et al.*, 1984; Millane & Arnott, 1986; Millane, 1989c)

$$I(\rho, \sigma) \simeq \frac{I_l(R_{hk})}{2\pi\alpha_0 l_{\text{lat}} l_{\text{axial}} \rho} \times \exp\left(-\left[\frac{(\rho - \rho_{hkl})^2}{2\beta_\rho^2} + \frac{(\sigma - \sigma_{hkl})^2}{2\beta_\sigma^2}\right]\right), \quad (4.5.2.27)$$

where $(\rho_{hkl}, \sigma_{hkl})$ are the polar coordinates of the reflection,

$$\beta_\rho^2 = \frac{l_{\text{lat}}^2 l_{\text{axial}}^2}{2\pi(l_{\text{lat}}^2 \sin^2 \sigma_{hkl} + l_{\text{axial}}^2 \cos^2 \sigma_{hkl})} \quad (4.5.2.28)$$

and

$$\beta_\sigma^2 = \alpha_0 + \frac{l_{\text{lat}}^2 l_{\text{axial}}^2}{2\pi\rho_{hkl}^2 (l_{\text{axial}}^2 \sin^2 \sigma_{hkl} + l_{\text{lat}}^2 \cos^2 \sigma_{hkl})}. \quad (4.5.2.29)$$

Reflections that have similar enough (R, Z) coordinates overlap severely with each other and are also included in the sum in equation (4.5.2.24). This is quite common in practice because a number of sets of reflections may have similar values of R_{hk} .

4.5.2.4.3. Random copolymers

Random copolymers are made up of a small number of different *kinds* of monomer, whose sequence along the polymer chain is not regular, but is random, or partially random. A particularly interesting class are synthetic polymers such as copolyesters that form a variety of liquid-crystalline phases and have useful mechanical properties (Biswas & Blackwell, 1988a). The structures of these materials have been studied quite extensively using X-ray fibre diffraction analysis. Because the molecules do not have an average c repeat, their diffraction patterns do not consist of equally spaced layer lines. However, as a result of the small number of distinct spacings associated with the monomers, diffracted intensity is concentrated about layer lines, but these are irregularly spaced (along Z) and are *aperiodic*. Since the molecule is not periodic, the basic theory of diffraction by helical molecules described in Section 4.5.2.3.2 does not apply in this case. Cylindrically averaged diffraction from random copolymers is described here. Related approaches have been described independently by Hendricks & Teller (1942) and Blackwell *et al.* (1984). Hendricks & Teller (1942) considered the rather general problem of diffraction by layered structures made up of different kinds of layers, the probability of a layer at a

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particular level depending on the layers present at adjacent levels. This is a one-dimensional disordered structure that can be used to describe a random copolymer. Blackwell and co-workers have developed a similar theory in terms of a one-dimensional paracrystalline model (Hosemann & Bagchi, 1962) for diffraction by random copolymers (Blackwell *et al.*, 1984; Biswas & Blackwell, 1988a), and this is the theory described here.

Consider a random copolymer made up of monomer units (residues) of N different types. Since the disorder is along the length of the polymer, some of the main characteristics of diffraction from such a molecule can be elucidated by studying the diffraction along the meridian of the diffraction pattern. The meridional diffraction is the intensity of the Fourier transform of the polymer chain projected onto the z axis and averaged over all possible monomer sequences. The diffraction pattern depends on the monomer (molar) compositions, denoted by p_i , the statistics of the monomer sequence (described by the probability of the different possible monomer pairs in this model) and the Fourier transform of the monomer units. Development of this model shows that the meridional diffracted intensity $I(Z)$ can be written in the form (Blackwell *et al.*, 1984; Biswas & Blackwell, 1988a; Schneider *et al.*, 1991)

$$I(Z) = \sum_i p_i |F_i(Z)|^2 + 2 \sum_i \sum_{j \neq i} \Re\{F_i(Z)F_j^*(Z)T_{ij}(Z)\}, \quad (4.5.2.30)$$

where the summations are over the different monomer types and $F_i(Z)$ is the axial Fourier transform of the i th monomer unit (each referenced to a common origin). The $T_{ij}(Z)$ are most conveniently described by defining them as the ij th element of an $N \times N$ matrix \mathbf{T} , which is given by

$$\mathbf{T} = \frac{\mathbf{P}\mathbf{M}\mathbf{X}(Z)}{\mathbf{I} - \mathbf{M}\mathbf{X}(Z)}, \quad (4.5.2.31)$$

where \mathbf{P} , \mathbf{M} , $\mathbf{X}(Z)$ and \mathbf{I} are $N \times N$ matrices. \mathbf{I} is the unit matrix and \mathbf{P} is a diagonal matrix with elements p_i . The elements M_{ij} of \mathbf{M} are the probabilities of forming ij monomer pairs and can be generated for different kinds of random sequence (*e.g.* chemical restrictions on the occurrence of particular monomer pairs, random chains, varying degrees of blockiness, tendency towards alternating sequences *etc.*) (Schneider *et al.*, 1991). The matrix $\mathbf{X}(Z)$ is diagonal with elements equal to $\langle \exp(i2\pi Z\zeta_i) \rangle$ where the ζ_i are the projected monomer lengths and the average is over all chain conformations.

Equation (4.5.2.30) can be used to calculate the meridional diffraction for a particular random copolymer. The most important result of such a calculation is that intensity maxima are spaced irregularly along the meridian. The positions of the maxima depend on the monomer proportions, the sequence statistics and the projected monomer lengths.

The full cylindrically averaged diffraction pattern, denoted by $I(R, Z)$, from a noncrystalline specimen containing oriented random copolymer chains can be calculated by replacing $F_i(Z)$ in equation (4.5.2.30) by $F_i(R, Z)$, *i.e.*

$$I(R, Z) = \sum_i p_i |F_i(R, Z)|^2 + 2 \sum_i \sum_{j \neq i} \Re\{F_i(R, Z)F_j^*(R, Z)T_{ij}(Z)\} \quad (4.5.2.32)$$

(Biswas & Blackwell, 1988a). Note that we write $I(R, Z)$ rather than $I_l(Z)$ since the pattern cannot be indexed on the basis of regularly spaced layer lines. The $F_i(R, Z)$ in equation (4.5.2.32) depend on the chain conformation, since this affects the range of monomer orientations and hence their average diffraction. Chivers & Blackwell (1985) have considered two extreme cases,

one corresponding to fixed conformations between monomers and the other corresponding to completely random conformations between monomers, and have derived expressions for the diffracted intensity in both cases. Equation (4.5.2.32) allows one to calculate the fibre diffraction pattern from an array of parallel random copolymers that exhibit no lateral ordering. The diffraction pattern consists of irregularly spaced layer lines whose spacings (in Z) are the same as those described above for the meridional maxima. Measurement of layer-line spacings and intensities and comparison with calculations based on the constituent monomers allows chain conformations to be estimated (Biswas & Blackwell, 1988a).

Diffraction patterns from liquid-crystalline random copolymers often contain sharp Bragg maxima on the layer lines. This indicates that, despite the random sequence and the possible dissimilarity of the component monomers, the chains are able to pack together in a regular way (Biswas & Blackwell, 1988b,c). Expressions that allow calculation of diffraction patterns for arrays of polymers with minimal registration, in which short, non-identical sequences form layers, have been derived (Biswas & Blackwell, 1988b,c). Calculation of diffracted intensities, coupled with molecular-mechanics modelling, allows chain conformations and packing to be investigated (Hofmann *et al.*, 1994).

4.5.2.4.4. Partially crystalline fibres

In this section we address disorder in the packing of the molecules in a polycrystalline fibre. The presence of disorder within the crystallites modifies the intensities of the Bragg reflections, as well as introducing continuous diffraction. The dominant effect, sometimes seen on fibre diffraction patterns (Stroud & Millane, 1995a), is for Bragg reflections to remain at low resolution but to be replaced by continuous diffraction at high resolution. There are two distinct cases to consider. The first is where the distortions at different lattice points in the crystallite are uncorrelated, and the second is where they are correlated.

Disorder within a crystallite in a polycrystalline fibre may consist of (1) deviations in the positions of the molecules (which are treated as rigid bodies) from their positions in a regular lattice, (2) rotations of the molecules about their molecular axes from their rotational positions in an ordered crystal, and (3) random orientations (up or down) of the molecules. The first of these is called *lattice disorder*, and the second and third are components of *substitution disorder*.

Uncorrelated disorder has been treated by a number of authors (Clark & Muus, 1962; Tanaka & Naya, 1969; Fraser & MacRae, 1973; Arnott, 1980). A rather complete model has been described by Millane & Stroud (1991) and Stroud & Millane (1995b), which is presented here. If the lattice and substitution disorders are independent, and the lattice and substitution distortions at different lattice sites are uncorrelated, then the cylindrically averaged layer-line intensities $I_l(R)$ diffracted from a fibre can be written as a sum of Bragg and diffuse (continuous) intensities (Tanaka & Naya, 1969):

$$I_l(R) = I_l^B(R) + I_l^D(R). \quad (4.5.2.33)$$

The profiles of the Bragg reflections are independent of the position of the reflection in reciprocal space. If the Cartesian components of the lattice distortions are independent, normally distributed, and the x and y components have equal variances, cylindrical averaging of the diffracted intensity can be performed analytically.

The lattice disorder consists of distortions of the two-dimensional lattice (in the lateral plane) into three-dimensional space, and in the *absence* of substitution disorder the Bragg component is given by (Stroud & Millane, 1995b)

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$$I_l^B(R) = I_l(R_{hk})w_{\text{lattice}}(R_{hk}, l/c) \quad (4.5.2.34)$$

where $I_l(R_{hk})$ is given by equation (4.5.2.24), the *lattice disorder weight*, $w_{\text{lattice}}(R, Z)$, is given by

$$w_{\text{lattice}}(R, Z) = \exp[-4\pi^2(R^2\sigma_{\text{lat}}^2 + Z^2\sigma_{\text{axial}}^2)], \quad (4.5.2.35)$$

where σ_{lat}^2 and σ_{axial}^2 are the variances of the lattice distortions normal ('lateral') and parallel ('axial') to the z axis, respectively. The diffuse component is given by

$$I_l^D(R) = (1/A_{\text{cryst}})I_l(R)[1 - w_{\text{lattice}}(R, l/c)], \quad (4.5.2.36)$$

where $I_l(R)$ is given by equation (4.5.2.17) and A_{cryst} is the average cross-sectional area of the crystallites. Inspection of equations (4.5.2.34) and (4.5.2.36) shows that the effect of the lattice disorder is to weight the amplitudes of the Bragg reflections down with increasing R and l , and to introduce a continuous intensity component whose amplitude increases with R and Z . Furthermore, the amplitude of the diffuse component relative to the Bragg component is inversely proportional to A_{cryst} , and therefore is not significant unless the crystallites are small.

If substitution disorder is also present, then equation (4.5.2.33) still applies but equations (4.5.2.34) and (4.5.2.36) are replaced by

$$I_l^B(R) = \left| \sum_n w_{nl} G_{nl}^2(R_{hk}) \exp[in(\psi_{hk} + \pi/2)] \right|^2 w_{\text{lattice}}(R_{hk}, l/c) \quad (4.5.2.37)$$

and

$$I_l^D(R) = (1/A_{\text{cryst}}) \sum_n |G_{nl}(R)|^2 [1 - |w_{nl}|^2 w_{\text{lattice}}(R, l/c)], \quad (4.5.2.38)$$

respectively, where the *substitution disorder weight*, w_{nl} , is given by

$$w_{nl} = \int_0^{c/2\pi} \int_0^z p(\varphi, z) \exp[i(2\pi z l/c - n\varphi)] d\varphi dz. \quad (4.5.2.39)$$

In equation (4.5.2.39), $p(\varphi, z)$ is the probability density function (p.d.f.) that describes the substitution disorder, *i.e.* the p.d.f. for a molecule being rotated by φ about and translated by z along the molecular axis relative to its position in the undistorted lattice. Inspection of equations (4.5.2.37) and (4.5.2.38) shows that the substitution disorder weights the different contributing Bessel terms differently. This can lead to quite complicated effects on the diffraction pattern for various kinds of substitution disorder, resulting in different distributions and amplitudes of Bragg and diffuse diffraction over the diffraction pattern (Stroud & Millane, 1995b). If one assumes either uniform or normal distributions for φ and z , then expressions can be obtained for the w_{nl} in terms of the variances of the distributions of φ and z (Stroud & Millane, 1995b). The cases where distortions in φ are correlated with distortions in z (*e.g.* 'screw disorder'), and directional (up and down) disorder, can also be accommodated. This model has been shown to be capable of predicting diffraction patterns which are in good agreement with those measured from some disordered polycrystalline fibres (Stroud & Millane, 1995a).

We consider now the case of correlated packing disorder. As a result of intermolecular contacts within a polycrystalline

specimen, it is possible that distortions at one lattice site will affect the degree of distortion at neighbouring sites. Coupling between distortions at different lattice sites can be included in the model of disorder by allowing the distortions at different lattice sites to be correlated. The effect of correlated distortions on diffraction patterns is that the diffracted intensity does not separate into Bragg and diffuse components as it does in the case of uncorrelated distortions [equation (4.5.2.33)]. The intensity can be described as being diffuse on the whole diffraction pattern, with (often broad) maxima occurring at some of the reciprocal-lattice points, but with no significant maxima at other reciprocal-lattice points. The widths of the profiles of the maxima generally increase with increasing resolution, whereas the widths of the Bragg maxima resulting from uncorrelated disorder as described above are independent of resolution. A broadening of diffraction maxima with increasing resolution and blending into continuous diffraction is sometimes seen on diffraction patterns from polycrystalline fibres, indicating the presence of correlated disorder (Stroud & Millane, 1996b).

Correlated lattice disorder consists of correlated distortions of the two-dimensional lattice into three-dimensional space. A flexible model of crystalline disorder is that based on the perturbed lattice approach (Welberry *et al.*, 1980). While formulating perturbed lattices with only nearest-neighbour interactions is complicated, a more tractable approach is to base the statistics on an imposed correlation field (de Graaf, 1989; Stroud & Millane, 1996a). This approach has been used to describe cylindrically averaged diffraction from polycrystalline fibres that contain correlated lattice disorder and uncorrelated substitution disorder (Stroud & Millane, 1996a,b), and is presented here.

To develop a flexible and tractable theory for diffraction from crystallites with correlated disorder, it is necessary to formulate the problem in real space. The size and shape of a crystallite in the xy (lateral) plane is described by a *shape function* $s_{\text{lat}}(\mathbf{r})$, where \mathbf{r} denotes the position vector in real space, which is equal to unity inside the crystallite and zero outside. The autocorrelation of the shape function, $t(\mathbf{r})$, is given by

$$t(\mathbf{r}) = \int s(\mathbf{r}') s(\mathbf{r} + \mathbf{r}') d\mathbf{r}'. \quad (4.5.2.40)$$

The correlations between the x components, and between the y components, of the distortions at any two lattice sites are taken to be identical. The correlations between distortion vectors are defined in terms of lateral, $\rho_{\text{lat}}(\mathbf{r})$, and axial, $\rho_{\text{axial}}(\mathbf{r})$, correlation fields such that the correlation coefficients between components of the distortions in the x (or y) and z directions, respectively, are equal to the correlation field evaluated for \mathbf{r} equal to the inter-site vector. Various functional forms for the correlation fields are possible, but exponential correlation functions are usually used (Stroud & Millane, 1996a). If $t(\mathbf{r})$ and the correlation fields are circularly symmetric, then cylindrical averaging of the diffracted intensity can be performed analytically.

For a polycrystalline fibre with correlated lattice disorder and uncorrelated substitution disorder, the diffracted intensity is given by (Stroud & Millane, 1996b)

$$\begin{aligned} I_l(R) = & \sum_{j,k} t(r_{jk}) w_{\text{lat}}(R, r_{jk}) w_{\text{axial}}(l/c, r_{jk}) \\ & \times \sum_{m,n} J_{n-m}(2\pi R r_{jk}) \Re \{ w_{ml} w_{nl}^* G_{ml}(R) G_{nl}^*(R) \\ & \times \exp[i(m-n)\varphi_{jk}] \} \end{aligned} \quad (4.5.2.41)$$

where $r = |\mathbf{r}|$, the sum over (j, k) is over all the sites of the undistorted lattice within the region occupied by the autocorrelation function, (r_{jk}, φ_{jk}) are the polar coordinates of the

