X-ray Scattering from a Discrete Helix with Cumulative Angular and Translational Disorders

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Abstract

X-ray scattering from a discrete helix possessing cumulative angular and translational disorders is studied by the Barakat model [Barakat (1987). *Acta Cryst.* A43, 45–49] assuming Gaussian distributions for random rotations and translations between subunits. This model is found to be identical to the paracrystalline model of the second kind. The intensity function shows that the intensity maximum decreases with increase in the Bessel order, whereas the peak breadth in the fiber direction and the intensity minimum increase.

Introduction

The scattering intensity for a helical structure having cumulative random angular disorder has been analyzed. Egelman & DeRosier (1982) derived the intensity function using an analogy with polymer statistics. Their equation is identical to the one after approximation derived by Barakat (1987), who assumed that the random rotations between subunits can be treated as zero-mean uncorrelated Gaussian random variables. The intensities given by the above authors, however, were restricted to the intensity maxima at the coordinates defined by the selection rule of helical diffraction. In the present communication, the Barakat (1987) model is analyzed to derive the total intensity distribution for a discrete helix having angular and translation cumulative disorders.

Intensity function with cumulative disorder

Consider a discrete helix possessing cumulative angular and translational disorders. The cylindrical coordinates at position j (r_j, φ_j, z_j, where $0 \leq j \leq N - 1$) may be given by

$$\varphi_j = j\Delta\varphi + \sum_{t=1}^{j} \partial_t,$$

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$$z_j = jP\Delta\varphi/2\pi + \sum_{t=1}^{j} \Delta_t$$

and

$$\Delta\varphi = 2\pi h/P, \quad r_j = r_0, \tag{1}$$

where P is the pitch of the helix, h is the subunit repeat of the helix, r_0 is the radius and ∂_t and Δ_t are the random variables describing the rotations and translations between the points (Egelman & DeRosier, 1982; Barakat, 1987). The origin was assigned to $r = r_0$, $\varphi = 0$ and $z = 0$. The structure factor in the cylindrical coordinates (Cochran, Crick & Vand, 1952) is given by

$$F(R,\Phi,Z) = \sum_{j=0}^{N-1} \sum_{n=-\infty}^{\infty} J_n(2\pi r_j R) \exp\left[in(\Phi + \pi/2)\right]$$

$$\times \exp\left[i(-n\varphi_j + 2\pi z_j Z)\right]. \tag{2}$$

With replacement of the cylindrical coordinates by the helical parameters (1) and after elimination of the cross terms of the different Bessel orders due to cylindrical averaging (Franklin & Klug, 1955), the intensity is given by

$$I(R,Z) = \sum_{n=-\infty}^{\infty} |J_n(2\pi r_0 R)|^2 \langle S(n,Z)\rangle,$$

where

$$\langle S(n,Z)\rangle = N + \sum_{j=0}^{N-1} \sum_{\substack{k=0 \\ j\neq k}}^{N-1} \exp\left[i(j-k)\Delta\varphi(PZ-n)\right]$$

$$\times \left\langle \exp\left[-in\left(\sum_{t=1}^{j} \partial_t - \sum_{t=1}^{k} \partial_t\right)\right]\right\rangle$$

$$\times \left\langle \exp\left[i2\pi Z\left(\sum_{t=1}^{j} \Delta_t - \sum_{t=1}^{k} \Delta_t\right)\right]\right\rangle \tag{3}$$

and $\langle\;\rangle$ denotes a statistical average. The statistical average for the angular disorder in (3) is given by

$$\left\langle \exp\left[-in\left(\sum_{t=1}^{j} \partial_t - \sum_{t=1}^{k} \partial_t\right)\right]\right\rangle$$

$$= \left\langle \exp\left(in \sum_{t=j+1}^{k} \partial_t \right) \right\rangle \quad \text{for } k > j$$

$$= \left\langle \exp\left(-in \sum_{t=k+1}^{j} \partial_t \right) \right\rangle \quad \text{for } k < j. \quad (4)$$

Similar equations are written for the translational disorder. With the multivariate characteristic function for zero-mean uncorrelated Gaussian random variables (Barakat, 1987),

$$\left\langle \exp\left(\pm ib \sum_{t=m_1}^{m_2} a_t \partial_t \right) \right\rangle$$

$$= \exp\left[-b^2 \langle \partial^2 \rangle \left(\sum_{t=m_1}^{m_2} a_t^2 \right)/2 \right], \quad (5)$$

where a_t and b are constants, ∂_t is a random variable and $\langle \partial^2 \rangle$ is the mean square displacement, the statistical averaging over the ∂_t in (4) and Δ_t leads to

$$\left\langle \exp\left[-in\left(\sum_{t=1}^{j} \partial_t - \sum_{t=1}^{k} \partial_t \right) \right] \right\rangle$$

$$\times \left\langle \exp\left[i2\pi Z\left(\sum_{t=1}^{j} \Delta_t - \sum_{t=1}^{k} \Delta_t \right) \right] \right\rangle$$

$$= \beta^{|j-k|} \quad \text{for } j \neq k, \quad (6)$$

where $\beta = \exp(-n^2 \langle \partial^2 \rangle/2 - 2\pi^2 Z^2 \langle \Delta^2 \rangle)$. Then, the intensity (3) is given by

$$\langle S(n,Z) \rangle$$
$$= N + \sum_{j=0}^{N-1} \sum_{\substack{k=0 \\ j \neq k}}^{N-1} \exp[i(j-k)\Delta\varphi(PZ-n)]\beta^{|j-k|}. \quad (7)$$

Replacement of $j - k$ by m and the double sum by a single sum in (7) gives

$$\langle S(n,Z) \rangle = N + \sum_{m=1}^{N-1} (N-m)\{\exp[im\Delta\varphi(PZ-n)]$$
$$+ \exp[-im\Delta\varphi(PZ-n)]\}\beta^m. \quad (8)$$

Use of a finite geometric series leads to

$$\langle S(n,Z) \rangle = \text{Re}[N(1+H)/(1-H)]$$
$$- 2\text{Re}[(H-H^{N+1})/(1-H)^2], \quad (9)$$

where $H = \beta \exp[i\Delta\varphi(PZ-n)]$ and Re refers to the real part of the function.

Equation (9) is given as a function of the continuous variable Z along the fiber direction. This is an identical form to the interference function for the one-dimensional paracrystalline lattice disorder of the second kind (Vainshtein, 1966). If $\Delta\varphi(PZ-n) = 2v\pi$ and $Z = (n/P) + (v/h)$, where n and v are integers (selection rule of helical diffraction), (9) has the same form as equation (3.2) of Barakat (1987). When N is

large, the second term is negligible, so (9) reduces to

$$\langle S(n,Z) \rangle = N(1 - \beta^2)$$

$$\times \{1 - 2\beta\cos[\Delta\varphi(PZ-n)] + \beta^2\}^{-1}. \quad (10)$$

When the cosine term is 1, $\langle S(n,Z) \rangle$ in (10) gives the intensity maximum $\langle S(n,Z) \rangle_{\text{max}} = N(1 + \beta)/(1 - \beta)$. When the cosine term is -1, i.e. $Z = (n/P) + (v/h) + 1/(2h)$, $\langle S(n,Z) \rangle$ in (10) gives the minimum intensity $\langle S(n,Z) \rangle_{\text{min}} = N(1 - \beta)/(1 + \beta)$. Since the integral area of the peak is N/h, the integral width (w) of the peak after subtraction of the area beneath the intensity minima is $(1 - \beta)/(2h)$. With no translational disorder, this reduces to $n^2 \langle \partial^2 \rangle/(4h)$ for a smaller angular deviation. Egelman & DeRosier (1982) reported a similar equation with $n^2 \langle \partial^2 \rangle/4$. For a finite number of subunits, the observed integral width squared, w_{obs}^2, is given by $B^2 + 1/(Nh)^2 + w^2$, where B and $1/(Nh)$ are the integral width of the direct beam and the coherent length of the perfect lattice, respectively. With the increase in the Bessel order, the intensity maximum decreases, whereas the peak breadth in the fiber direction and the intensity minimum increase. When the intensity maximum is 1.2 times larger than the intensity minimum, the peak may no longer be detected (Vainshtein, 1966). This occurs at $n^2 \partial^2 = 6.18$ when there is no translational disorder.

Intensity function with noncumulative disorder

If the angular and translational disorders are not cumulative (for an independent oscillator model of thermal disorder or static disorder of the first kind), the β^m in (8) may be replaced by β^2 (see also Worthington & Elliott, 1989). Then, the intensity is given by

$$\langle S(n,Z) \rangle = S_0(n,Z)\beta^2 + N(1 - \beta^2), \quad (11)$$

where $S_0(n,Z)$ is the intensity of the perfect lattice and is given by

$$\sin^2[N\Delta\varphi(PZ-n)/2]/\sin^2[\Delta\varphi(PZ-n)/2].$$

When the displacements are small, the exponential term in β reduces to

$$(1 - n^2\langle\partial^2\rangle/2)(1 - 2\pi^2 Z^2\langle\Delta^2\rangle).$$

Stokes & DeRosier (1987) reported a similar formula for the noncumulative disorders, which contains a proportional factor N^2 arising from the intensity maximum of the $S_0(n,Z)$ term but does not include the $N(1 - \beta^2)$ term.

Discussion

The Barakat (1987) model of X-ray scattering of a discrete helix with a cumulative angular disorder is

based on the multivariate characteristic function for zero-mean uncorrelated Gaussian random variables. We have shown here that this model can lead to the intensity formula [(8) and (9)] analogous to that of the paracrystalline lattice (Vainshtein, 1966). We included the cumulative disorder parameter in the structure factor (2) and derived the intensity function whereas Worthington & Elliott (1989) defined the paracrystalline disorder in the autocorrelation function and calculated its Fourier transform. The intensity in the latter was not given in a closed form and was not explicity dependent on the Bessel order n for an angular disorder. Although Worthington & Elliott (1989) indicated by computer simulation that the n dependence of angular disorder is inherent in their formulation, the relation between their approach and ours has not yet been derived.

The measurement of a cumulative angular disorder has been previously reported for the actin filament as 12° per subunit (Stokes & DeRosier, 1987). These authors, on the basis of the theory of Egelman & DeRosier (1982), used optical diffraction patterns from electron micrographs for a negatively stained filament. In order to determine a disorder parameter, the intensity of the layer line was plotted as a function of the number of lattice points. Their measured value, however, appeared to disagree with the measured bending flexibility (Erickson, 1989). It will be beneficial therefore to use X-ray diffraction intensities instead of optical diffraction in order to determine the angular disorder of nontreated and nonstaining specimens. The procedure of Stokes & DeRosier (1987), however, will not be used because it requires multiple X-ray diffraction patterns from fibers having distinctly different N values. The new intensity function described in this text shows the way to measure the angular disorder from a single X-ray diffraction pattern. As first suggested by Egelman & DeRosier (1982), the broadening of the intensity along the fiber axis increases with the increase in the Bessel order n and the angular disorder. By comparing the breadths or the intensity profiles [by using (9)] of the layer lines having differ-ent Bessel order n, the angular disorder will be determined. Tajima, Kamiya & Seto (1983) noted that, as the theory predicts, actin layer lines of a molluscan smooth muscle become broader with the increase in the absolute value of the Bessel order.

The effects of disorder on fiber diffraction patterns have recently been analyzed (Millane & Stroud, 1991). The disorders refer to the lattice disorder (the first kind) and the variations of a filament positioned at that lattice point owing to the Clark–Muus-type angular, translational and screw disorders (Clark & Muus, 1962; Tanaka & Naya, 1969). While we have studied here the cumulative disorder within a helix, these workers analyzed the noncumulative disorder.

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