Short Communications

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Patterson transforms and the interpretation of X-ray scattering from fibers.

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MacGillavry & Bruins (1948) have shown how X-ray analysis of the structure of fibers may be aided by computation of a suitable Patterson transform. They assume, however, that the fiber structure possesses strict periodicity in the direction of the fiber axis. Many fibers of interest fail to meet this condition, as evidenced by great diffuseness of their X-ray scattering in the axial direction as well as the equatorial, and the absence of well-defined layer lines (Astbury, 1943). We wish to point out that these structures can also be analyzed by a modification of the method of MacGillavry & Bruins, and, furthermore, to formulate the analyzing process in a somewhat more suitable manner than they have done. We refer to their paper for description of the experimental arrangement and definition of all symbols except those newly introduced.

We assume that the fiber structure possesses no long-range periodicity. The X-ray scattering determines the Patterson function (or auto-correlation function of electron density), $\phi(\mathbf{y})$ (MacGillavry & Bruins, 1948, equation (2)), and this is a continuous function of both z and x. For $|\mathbf{y}|$ large compared with the dimensions of the microstructure within the fibers $\phi(y)$ is sensibly constant, and equal to ρ_0^2, where ρ_0 is the mean density of electrons in the fibrous material. The observed scattered intensity, $H(\mathbf{h})$, is then given by

$$H(\mathbf{h}) = V\int_{\mathbf{y}} [\phi(\mathbf{y}) - \rho_0^2] \exp(2\pi i \mathbf{h}.\mathbf{y})\, d\tau_y, \qquad (1)$$

except in the nearly straightforward direction, where scattered radiation cannot be distinguished from the main beam anyway. This subtraction of ρ_0^2 is justified in the same way as the equivalent step in the usual theory of liquid diffraction, and it is needed for the same reasons as in that theory.

In the same way as in the paper of MacGillavry & Bruins, equation (1) may then be converted to

$$H(\zeta, \xi) = 2\pi V \int_z \int_x [\phi(z,x) - \rho_0^2]\, I_0(2\pi\xi x) \exp(2\pi i \zeta z)\, x\, dx\, dz.$$

This integral equation for $\phi(z, x)$ may be immediately solved by a two-dimensional Fourier–Bessel inversion theorem to give

$$\phi(z,x) - \rho_0^2 = \frac{2\pi}{V}\int_\zeta \int_\xi H(\zeta,\xi)\, I_0(2\pi\xi x) \exp(-2\pi i\zeta z)\, \xi\, d\xi\, d\zeta. \qquad (2)$$

Transforming from electron units to absolute units of scattered intensity, assuming unpolarized incident radiation; letting θ be the scattering angle, R the distance from sample to point of observation, H_0 the intensity of the incident beam at the sample; and giving e, m and c their usual meanings, equation (2) yields

$$\phi(z,x) = \rho_0^2 + \frac{8\pi m^2 c^4}{VH_0 e^4}\int_0^\infty \int_0^\infty \frac{H(\zeta,\xi)\, R^2}{1+\cos^2\theta} \times I_0(2\pi\xi x)\cos(2\pi\zeta z)\, \xi\, d\xi\, d\zeta. \qquad (3)$$

In practice, an incoherent scattering correction will be needed before (3) is applied, and this may be made in the same way as in the usual liquid diffraction theory. One needs to know what elements compose the fibrous substance and what the percentage by weight is of each, and must make a measurement of scattered intensity at an angle so large that all atoms are scattering independently. In this process, the value of VH_0 may also be worked out.

There is one case, perhaps of considerable practical importance, in which the integration of equation (3) may be much simplified. If there is structure in the fiber of dimensions much larger than atomic, this will provide scattering which is confined to small angles. By ignoring all scattering except this small-angle scattering in the integral of (3), one finds an auto-correlation function which reveals this larger-scale structure without any details of an atomic scale. More strictly, this is the auto-correlation function for an electron density differing from the actual density in being smoothed (by averaging) over distances of the order of atomic dimensions only. Suppose the scattered radiation is detected on a flat plate perpendicular to the incident beam and displaced from the sample by a distance R_0. Let Y and Z be Cartesian coordinates of points in the detecting plate, measured from an origin which is the point of intersection in the plate of the unscattered beam, and let the Z axis be parallel to the fiber axis. Let $H(Y, Z)$ be the scattered intensity at Y, Z. One readily finds, then, the small-angle approximation to equation (3) (in which $H(Y, Z)$ must be set equal to zero at large angles)

$$\phi(z,x) \simeq \rho_0^2 + \frac{4\pi m^2 c^4}{VH_0 e^4 \lambda^3 R_0}\int_0^\infty \int_0^\infty H(Y,Z) \times I_0\left(\frac{2\pi x Y}{\lambda R_0}\right)\cos\left(\frac{2\pi z Z}{\lambda R_0}\right) Y\, dY\, dZ,$$

and which determines only the above-mentioned larger-scale structure of the fiber.

The writer is indebted to Dr A. N. J. Heyn for bringing this problem to his attention.

References

Astbury, W. T. (1943). *Textile Fibers Under the X-Rays.* London: Imperial Chemical Industries.

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