Short Communications

Contributions intended for publication under this heading should be expressly so marked; they should not exceed about 500 words; they should be forwarded in the usual way to the appropriate Co-editor; they will be published as speedily as possible; and proofs will not generally be submitted to authors. Publication will be quicker if the contributions are without illustrations.

Acta Cryst. (1959). **12**, 171

Scattering from an infinite elliptical cylinder.

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(*Received* 10 *June* 1958)

The low-angle equatorial region of the X-ray diffraction pattern from α-keratin is dominated by three maxima, centered at 86, 45 and 28 Å. We have recently attempted to explain this observation in terms of a model consisting of irregularly close-packed cylindrical microfibrils with an average inter-particle distance of 100 Å (Fraser & MacRae, 1958).

The normalized scattering from a circular cylinder of radius R can be expressed (Oster & Riley, 1952) by

$$F^2(r^*) = \left[\frac{2J_1(2\pi r^*R)}{2\pi r^*R}\right]^2, \quad (1)$$

in which J_1 is a Bessel function of order one and r^* is a radial coordinate in reciprocal space of magnitude $2 \sin \theta/\lambda$, where 2θ is the scattering angle. If the microfibrils are assumed to have a radius $R = 35$ Å it is found that the origin peak of $F^2(r^*)$ still has considerable magnitude at a value of r^* corresponding to the 86 Å reflection, and that the next two maxima in the calculated curve occur close to the r^* values for the observed 45 and 28 Å reflections.

When osmium is deposited in the structure (Fraser & MacRae, 1957) these three reflections are considerably increased in intensity. No such intensification is, however, observed in that region of the pattern where it would be predicted from the occurrence of a fourth maximum in the function $F^2(r^*)$ for a circular cylinder.

We have found that one way that this effect can be accounted for is by assuming that the diffracting cylinder is elliptical rather than circular. In this case expression (1) becomes:

$$F^2(r^*) = \frac{1}{2\pi}\int_0^{2\pi}\left[\frac{2J_1(2\pi r^*R(K^2\cos^2\alpha+\sin^2\alpha)^{\frac{1}{2}})}{2\pi r^*R(K^2\cos^2\alpha+\sin^2\alpha)^{\frac{1}{2}}}\right]^2 d\alpha\,, \quad (2)$$

where R is now the semi-minor axis and K is the axial ratio of the ellipse.

Values of $F^2(r^*)$ at 0·001 intervals in r^* were calculated on the SILLIAC electronic digital computer. A subroutine from the computer library was used to calculate the first-order Bessel function $J_1(x)$ for $x > \frac{1}{2}$ via the expressions

$$J_1(x) = (2/\pi x)^{\frac{1}{2}}\,[\sin(x-\pi/4)+(3/8x)\sin(x+\pi/4)] \quad \text{for } x \geq 16$$

and

$$J_1(x) = x/2\sum_{s=0}^{N}(-1)^s(x/2)^{2s}/s!(s+1)! \quad \text{for } \tfrac{1}{2} < x < 16.$$

For $x \leq \frac{1}{2}$ the approximation

$$J_1(x)/x = \tfrac{1}{2}\sum_{s=0}^{2}(-1)^s(x/2)^{2s}/s!(s+1)!$$

was used directly. The numerical integration was carried out by Simpson's Rule at 3° intervals over one quadrant. The results were correct to $\pm 0{\cdot}0001$.

For $R = 35$ Å the results obtained for values of K = 1, 1·05, 1·1, 1·15, and 1·2 are shown graphically in

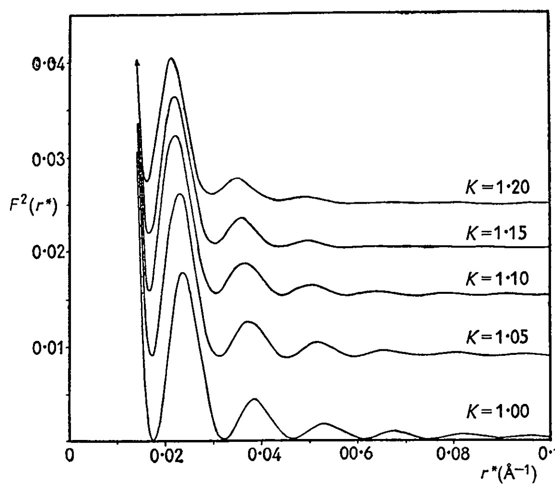

Fig. 1. Normalized equatorial scattering from elliptical cylinders of varying axial ratios (K). For clarity the curves for different axial ratios are displaced vertically. The scale of $F^2(r^*)$ refers to the curve for $K = 0$.

Fig. 1, and it can be seen that for the last value, the fourth and all succeeding maxima are virtually eliminated.

We are grateful to the Director and staff of the Adolph Basser Computing Laboratory, University of Sydney, for the provision of computing facilities.

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