all terms whose spacing was greater than 10 Å. The results are shown in Fig. 2. The two curves correspond to unsharpened data (the dashed line) and sharpened data (the continuous line).

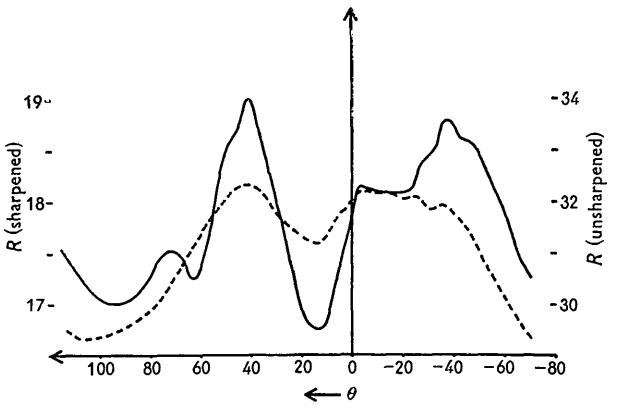

Fig. 2. Rotation function when the [010] direction of horse oxyhaemoglobin is rotated by the angle θ about the [110] human oxyhaemoglobin Patterson. The shaded line is the unsharpened 6 Å rotation function, while the full line represents the data sharpened by omitting all terms with spacing greater than 10 Å.

A check on the level of the background of the rotation function was made by calculating 28 points for values of $\varkappa$ between 0° and 360° in 10° to 15° increments, when $\psi = 35{\cdot}5°$, $\varphi = 54{\cdot}5°$. This section contains the peak at $\theta = 40°$. By averaging the rotation function values, omitting the points which lay within 7·5° of the large peak, the mean value (corresponding to the persistent origin overlap) of R was found to be 17·6 units, and the r.m.s. deviation from the mean was 0·4 units. Thus the peak at $\theta = 40°$, with $R = 18{\cdot}97$, is 3·6 standard deviations above the mean. The second largest peak was less than two standard deviations above background.

Fig. 2 shows two peaks, one of the peaks being rather broader and lower than the other peak. These two peaks arise as a consequence of the pseudo 222 symmetry of the haemoglobin molecule. That is, while one peak corresponds to the superposition of the self-Pattersons of an α onto an α chain and of a β onto a β chain, the other peak corresponds to the superposition of the self-Pattersons of the α onto β and β onto α chains. If the haemoglobin molecules were to contain exact 222 symmetry then the two peaks would be of the same height. Furthermore, in the Patterson the directions of the two different pseudo twofold axes of the molecule must make equal and opposite angles with the tetragonal fourfold axis. Thus if the monoclinic Patterson is positioned on top of the tetragonal Patterson, so as to superimpose the corresponding pseudo twofold directions, there will be good agreement, whereas at an equal and opposite angle with the tetragonal c axis the agreement will not be as good. As the arbitrary reference line from which θ is measured in the monoclinic system coincides to within 5° of the molecular pseudo twofold axis, the two peaks should occur at $\pm\theta$, approximately. Fig. 2 shows the two peaks to be at $\theta = 40°$ (sharp) and $-37°$ (broad).

The agreement of the position of the peak at θ with that at $-\theta$ to within 3°, and the agreement with the results of Perutz (1953) who showed from optical birefringence experiments that θ must be either 35° or —15° establishes the relative orientation of the two molecules as lying between $\theta = 35°$ and 40°. The large size of the peak at $\theta = -37°$ might suggest that the superposition of the 222 symmetrical parts of the molecular Pattersons agree better than the non-symmetrical parts.

We are grateful for discussions with Dr. M. F. Perutz, and to Dr. Hilary Muirhead for allowing us to use her human oxyhaemoglobin data. All calculations were made on the IBM 7090 computer, assisted by the IBM Endowed Time scheme.

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The Fourier transform of an assembly of helices.

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Many biological polymers have a helical conformation and it is possible to calculate the Fourier transform of a single molecule from the expressions of Cochran, Crick & Vand (1952) and Klug, Crick & Wyckoff (1958). It is evident however, from recent X-ray studies of the fibrous proteins α-keratin (Fraser, MacRae & Rogers, 1962) and paramyosin (Cohen & Holmes, 1963) that account must be taken of the interference which occurs as a result of the helices being assembled into bundles or fibrils. The present note describes a method of calculating the cylindrically averaged intensity from an assembly of N helices in which the helix axes are parallel to a unique direction Oz (the fibre axis). Following Klug *et al.*, we may express the transform of a right-handed helical molecule with helix axis coincident with Oz as

$$F_0(R, \psi, l/c) = \sum_n G_{n,l}(R) \exp\,[in(\psi + \tfrac{1}{2}\pi)] \qquad (1a)$$

where

$$G_{n,l}(R) = \sum_j f_j J_n(2\pi R r_j) \exp\,[i(-n\varphi_j + 2\pi l z_j/c)]. \qquad (1b)$$

The notation is that used by Klug *et al.* and the summation in (1*a*) extends over the values of n which satisfy the relation $l=tn+um$ and the summation in (1*b*) extends over the atoms in a set. In many instances (*e.g.* the α-helix) only one term is needed in (1*a*) for a particular value of l; this is the case considered here.

If a convenient axis Oz is chosen within the fibril we may suppose this to coincide with the helix axis of an imaginary reference molecule having some arbitrary rotation about Oz and displacement along Oz. The Fourier transform, F_o, of this reference molecule may then be calculated by expression (1). Each molecule in the fibril may generated from the reference molecule by a rotation α_v about Oz, a displacement z_v parallel to Oz and a displacement normal to Oz of magnitude r_v and azimuth φ_v. The transform of the fibril is thus

$$F(R, \psi, l/c) = \sum_v F_o(R, \psi-\alpha_v, l/c) \exp\{2\pi i[Rr_v \cos(\psi-\varphi_v)+\zeta z_v]\} \quad (2)$$

where the summation extends over the N molecules in the fibril and does not, of course, include the imaginary reference molecule. A similar expression, in cartesian coordinates, is implied in Section 4 of Cochran *et al.* (1952).

The intensity transform for the fibril is, from (1) and (2),

$$FF^*(R, \psi, l/c) = |G_{n,l}(R)|^2 \sum_v \sum_w \exp\{i[-n\alpha_{vw} + 2\pi Rr_{vw}\cos(\psi-\varphi_{vw})+2\pi\zeta z_{vw}]\} \quad (3)$$

where $\alpha_{vw}=\alpha_v-\alpha_w$, $z_{vw}=z_v-z_w$, r_{vw} is the magnitude of a vector normal to Oz joining the axes of the vth and wth molecules and φ_{vw} is the angle between this vector and the plane $\psi=0$. In most instances the angular dependence of (3) is of no interest and the observable intensity is proportional to the cylindrically averaged value

$$\langle FF^*(R, \psi, l/c)\rangle_\psi = \int_0^{2\pi} FF^*(R, \psi, l/c)d\psi/2\pi. \quad (4a)$$

From (3), (4*a*) and the identity

$$J_o(x) = \int_0^{2\pi} \exp(ix\cos\theta)d\theta/2\pi$$

we obtain

$$\langle FF^*(R, \psi, l/c)\rangle_\psi = |G_{n,l}(R)|^2 \sum_v \sum_w J_o(2\pi Rr_{vw}) \cos(-n\alpha_{vw}+2\pi\zeta z_{vw}) \quad (4b)$$

It may be noted that for $l=n=\zeta=0$ the expression reduces to that derived by Oster & Riley (1952) for the equatorial scattering from assemblies of cylindrically symmetrical systems. Also for $N=1$ (4*b*) reduces to $|G_{n,l}(R)|^2$ which is the result given by Klug *et al.* (1958) for a single molecule and a single value of n. The effect of interference between helical molecules in a fibril is thus the introduction of a double summation as in (4*b*).

This double summation implies the calculation of N^2 terms but in practice the maximum number required is $N(N-1)/2$ at most as $\alpha_{vw}=-\alpha_{wv}$ and $z_{vw}=-z_{wv}$ and (4*b*) simplifies to

$$\langle FF^*(R, \psi, l/c)\rangle_\psi = |G_{n,l}(R)|^2\{N+2\sum_{v=1}^{N}\sum_{w=v+1}^{N} J_o(2\pi Rr_{vw}) \times \cos(-n\alpha_{vw}+2\pi\zeta z_{vw})\} \quad (5)$$

If, as frequently is the case, the molecules are symmetrically arranged within the fibril the number of terms in the double summation which need to be calculated is quite small.

We have shown elsewhere (Fraser, MacRae & Miller, 1964) that the Fourier transform of the coiled-coil model for α-fibrous proteins proposed by Crick (1953) may be written in the form

$$F(R, \psi, l/c) = G(R, m, \lambda)\exp[i\lambda(\psi+\tfrac{1}{2}\pi)] \quad (6)$$

where $l/c=\lambda/P+m/h$, P is the pitch of the major helix, h is the axial rise per seven residues and only a single combination of m and λ is needed for any particular l. $G(R, m, \lambda)$ is a complex number independent of ψ and so (6) is formally similar to (1). The analysis leading to (5) is thus equally valid in this case. Further it has been shown that when a number of coiled-coil structures are wound around a common axis to form a rope the Fourier transform of the rope can also be expressed in a form similar to (6) (Fraser *et al.*, 1964) and so (5) may also be applied to fibrils containing assemblies of coiled-coil ropes.

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A comment on centroid truncation procedures.

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A description of a truncation procedure for the determination of the centroid position of an X-ray diffraction line, and an account of the advantage of this procedure in dealing with the difficulties introduced by satellite lines, have recently been published (Taylor, Mack & Parrish, 1963; Parrish, Mack & Taylor, 1963).

A similar procedure, together with the results obtained when it is used to determine lattice parameters, has