P_C2/m and C_c2/m. It follows that the resulting magnetic space groups allowed by the experimental data are P_A2_1/c and C_c2/c.

It is convenient to write the space group P_A2_1/c as P_C2_1/a, because the latter notation corresponds to the convential choice of axes for the space group $C2/m$. The space group P_C2_1/a requires a magnetic unit cell with the same size as the X-ray unit cell and with an anticentre in the *ab* plane (Fig. 2). The unit cell belonging to C_c2/c is twice as large as the X-ray unit cell. Depending on the choice of the *a* axis one obtains either a unit cell with a normal centre and an antitranslation in the **c** direction or a unit cell with an anticenter in the *ab* plane and an antitranslation in the **c** direction.

The following rules apply to the arrangements of magnetic moments, prescribed by either of the two allowed magnetic space groups. The iron ions of type I are situated at the intersection of an antimirror plane and a twofold anti-axis. Their magnetic moments are therefore parallel to the *ac* plane; the direction in the *ac* plane cannot be determined on the basis of the experimental data. The iron ions of type II are situated on twofold anti-axes on either side of an antimirror plane. The magnetic moments of the two members of a pair of these irons ions are then mutually parallel. Their common direction is parallel to the *ac* plane. Again, the direction in the *ac* plane is not known.

The magnetic structure reported in this paper seems to be confirmed by recent susceptibility measurements (Meijer, van den Handel & Frikkee, 1967).

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A Modified Theory for the Fourier Transform for a Coiled-Coil

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Published theory for the Fourier transform of a coiled-coil is shown to correspond to a filament with variable line density. A modified expression representing the Fourier transform of a close approximation to a coiled-coil of constant line density is described.

A coiled-coil (super-helix) structure has recently been suggested for nucleohistone (Pardon & Wilkins, 1967) and Fourier transform calculations made to test its feasibility. The theory originally used in the calculations was that previously applied to the coiled-coil model for α-keratin (Crick, 1953*a*,*b*; Lang, 1956; Ramachandran, 1960; Fraser, MacRae & Miller, 1964). However, at an early stage in the calculations this theory was found to represent a filament with variable line density and therefore proved unsuitable. A modified theory for the Fourier transform of a coiled-coil, which represents a close approximation to a filament of constant line density, is outlined in this paper.

The previously published expression representing the Fourier transform of a continuous 'infinitely thin wire of electron density' constrained to form a coiled-coil is:

$$C(R,\psi,l/c)=\sum_p\sum_q\sum_s\sum_d J_p(2\pi Rr_0)\,.\,J_q(2\pi R\bar{r}_1)\,.\,\times J_d(2\pi R\Delta)\,.\,J_s(2\pi(l/c)r_1\sin\alpha)\,.\,E\,,$$

where

$$E=\exp[i(p(\psi-\varphi_0+\tfrac{1}{2}\pi)+q(-\psi+\varphi_0+\varphi_1+\tfrac{1}{2}\pi)+s(\pi+\varphi_1)+d(\psi+\varphi_1-\varphi_0+\tfrac{1}{2}\pi)+2\pi z_0l/c)\,, \quad (1)$$

subject to

$$N_0p+(N_1-N_0)q+(N_1+N_0)d+N_1s=l\,,$$

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where

r_0 = major helix radius
r_1 = minor helix radius
$\bar{r}_1 = r_1(1+\cos\alpha)/2$
$\Delta = r_1(1-\cos\alpha)/2$
$\tan\alpha = 2\pi r_0 N_0/c$
$R, \psi, l/c$ are cylindrical coordinates in reciprocal space.

The following considerations indicate that this expression does not represent the Fourier transform of a coiled-coil of constant line density.

Consider a line distribution along a curve defined in terms of a parameter t by the equations:

$$x = x_0(t) \quad y = y_0(t) \quad z = z_0(t) .$$

If t_1, t_2 are the parameters corresponding to the end points of the line distribution, the Fourier transform of the distribution is:

$$F(u,v,w) = \int_{t_1}^{t_2} \varrho(t) \exp[2\pi i(ux_0 + vy_0 + wz_0)]dt ,$$

where $\varrho(t)$ is the line density in terms of parameter t, such that the total weight of the filament between t_1 and t_2 becomes

$$w = \int_{t_1}^{t_2} \varrho(t)dt .$$

The actual line density in terms of the parameter s, the length of the arc of the curve is:

$$\frac{dw}{ds} = \frac{\frac{dw}{dt}}{\frac{ds}{dt}} .$$

For the transform to correspond to that of a uniform line density along the curve, $dw/ds = k$, where k is a constant

$$i.e.\ \varrho(t) = \frac{dw}{dt} = k\frac{ds}{dt} .$$

For the coiled-coil defined previously in terms of the parameter t (Crick, 1953*a*):

$$\frac{ds}{dt} = [A + B\cos(\gamma w_0 t - \theta) + C\cos^2(\gamma w_0 t - \theta)]^{\frac{1}{2}} ,$$

where

$$\begin{aligned} A &= [r_0^2 + \bar{r}_1^2(1+\gamma)^2 + \Delta^2(1-\gamma)^2 + (P/2\pi)^2 \\ &\quad - 2\bar{r}_1\Delta(1-\gamma^2)]w_0^2 \qquad (2) \\ B &= [2r_0 r_1(1+\gamma\cos\alpha) - Pr_1\gamma\sin\alpha/\pi]w_0^2 \\ C &= [r_1^2\gamma^2\sin^2\alpha + 4\bar{r}_1\Delta(1-\gamma^2)]w_0^2 ; \end{aligned}$$

γ defines the ratio of the number of turns in the minor helix to those in the major helix so that $w_1/w_0 = N_1/N_0 = \gamma$. P = major helix pitch.

Hence for the coiled-coil defined by the parameter t, ds/dt is not constant. As a term representing $\varrho(t)$ was not included in the expression for the transform [equation (1)] the expression does not correspond to a filament of constant line density. Lang (1956) in his expression for a generalized transform includes a term A_0 representing the line density and indicates that the variation can be expressed in terms of the Fourier series

$$A_0 = \sum_{p=-\infty}^{p=\infty} \varrho_p \exp(-2\pi ipt/t_m) .$$

However, when Lang applies this general theory to the Fourier transform of a coiled-coil he assumes that the line density function $\varrho(t)$ does not vary with t.

This error in the theory had been independently found by Patterson (private communication) who suggested that the following methods lend themselves to a solution of the problem:

(*a*) Redefine the coiled-coil in terms of a new parameter t chosen so that ds/dt is constant.

(*b*) Modify the expression given in equations (1) by including terms $\varrho_p(t)$ as in Lang's generalized theory, where $\varrho_p(t)$ are coefficients of the Fourier series for ds/dt.

Neither of these alternatives was possible, but the problem has been approximately solved by using the following Fourier series, which is an approximation to ds/dt:

$$\left(\frac{ds}{dt}\right)' = A' + B'\cos(\gamma w_0 t - \theta) ,$$

where

$$\begin{aligned} 2A' &= (A+B+C)^{\frac{1}{2}} + (A-B+C)^{\frac{1}{2}} \\ 2B' &= (A+B+C)^{\frac{1}{2}} - (A-B+C)^{\frac{1}{2}} , \end{aligned}$$

A, B and C being defined in equation (2).

The close agreement between this expression and ds/dt for a coiled-coil typical of the models that have been studied as a possible model for nucleohistone (Pardon & Wilkins, 1967) is shown in Table 1. A closer approximation could have been obtained by including a third term $C'\cos 2(\gamma w_0 t - \theta)$, but for the models under consideration this was not found to be necessary.

Table 1. *The variation of ds/dt and (ds/dt)′ with wt for a coiled-coil, with dimensions*: $P = 120$, $r_0 = 50$, $r_1 = 40$ Å, $N_0/N_1 = 1$

wt	*ds/dt*	*(ds/dt)′*
0	94·46	94·46
10	93·91	93·97
20	92·29	92·53
30	89·65	90·16
40	86·08	86·96
50	81·69	83·01
60	76·65	78·44
70	71·11	73·37
80	65·29	67·98
90	59·38	62·41
100	53·60	56·85
110	48·18	51·45
120	43·30	46·39
130	39·14	41·82
140	35·80	37·87
150	33·31	34·67
160	31·63	32·31
170	30·69	30·87
180	30·38	30·38

The modified expression for the Fourier transform after inclusion of the line density correction term becomes:

$$C(R,\psi,l/c)=\sum_m\sum_p\sum_d\sum_q\sum_s \varrho_m \,.\, J_p(2\pi R r_0)\,.\, J_d(2\pi R\Delta)\,. \times J_q(2\pi R\bar{r}_1)\,.\, J_s(2\pi r_1 \sin\alpha\,.\, l/c)E\,, \quad (3)$$

where

$$E=\exp[i(p(\psi-\varphi_0+\tfrac{1}{2}\pi)+q(-\psi+\varphi_0+\varphi_1+\tfrac{1}{2}\pi) +d(\psi+\varphi_1-\varphi_0+\tfrac{1}{2}\pi)+s(\pi+\varphi_1)+2\pi z_0 l/c)\,,$$

subject to

$$N_0p+(N_1-N_0)q+(N_1+N_0)d+N_1s=l+m$$

where

$$\varrho_0=A'\,.\,\varrho_1=\varrho_{-1}=B'$$

and all ϱ_i for $|i|>1$ are zero.

The theory has been checked by comparing results obtained from the expression of equation (3) with the optical diffraction pattern obtained from a mask which corresponded to a projection of a coiled-coil of constant line density and also, following a suggestion by Dr A. R. Stokes, by computing the Fourier transform obtained by a direct substitution of the coordinates of points (x_i,y_i,z_i), spaced at small equal increments in Δs along the coiled-coil, into the expression

$$C(R,\psi,l/c)=\sum_{i=1}^{N}\exp[2\pi i(Xx_i+Yy_i+Zz_i)]\,.$$

In both cases a good agreement was obtained (Pardon, 1966).

Discussion

It has been shown that for models in which the original helix suffers appreciable distortion in forming a coiled-coil, the filament generated with the cartesian coordinate system adopted by Crick (1953) does not approximate to a filament of constant line density. The modified theory outlined above represents the Fourier transform of a model with much less variation in line density; this has been used in calculations for groups consisting of various numbers of coiled-coils packed coaxially. The theory has been found to be very satisfactory for models in which $P=120$ Å, $r_0=50$ Å, 30 Å $\leq r_1 \leq 40$ Å and where N_0/N_1 varied from 1 to 3.

If the original simple helix undergoes little distortion in forming the coiled-coil, as in the case considered by Crick (1953*a*,*b*), then the differences between the Fourier transforms calculated from the original theory and those from the modified theory are small. It seems probable that the original theory is sufficiently accurate for a model such as has been studied for α-keratin.

The proposed super-helical model for nucleohistone and supporting experimental evidence has been recently described by Pardon, Wilkins & Richards (1967).

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The Structure of the *M'*- Phase of $YTaO_4$, a Third Fergusonite Polymorph

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The *M'* phase of fergusonite is closely related to the other known monoclinic form (*M* phase), except that it has a halved *b* axis and its space group is $P2/a$ instead of $I2$. The structure of the *M'* phase has been determined for $YTaO_4$ from three-dimensional diffractometer data, and its relationship to the other polymorphs is discussed. The lattice parameters of *M'*-$YTaO_4$ are: $a=5{\cdot}292$, $b=5{\cdot}451$, $c=5{\cdot}110$ Å, $\beta=96{\cdot}44°$, $Z=2$.

Introduction

Using a natural fergusonite (impure $YNbO_4$), Komkov (1959) determined the structure of the high-temperature form to be that of scheelite, space group $I4_1/a$, with oxygen coordinates close to those of $CaWO_4$ (Kay, Frazer & Almodovar, 1964), and that of the low-temperature form to be a distorted scheelite, space group $I2$. The two forms, which will be referred to as the *T* phase and the *M* phase, respectively, are related by