advantage of the modulus projection for solving complex structures, but there is a slight compensation in the reciprocal relationship: namely that if overlap leads to a small peak height in a modulus projection, the contributions of these two overlapping atoms to the structure amplitudes of that particular layer are correspondingly small. Also, it is somewhat rare for complete overlap to occur fortuitously, and when initiating a crystal analysis with modulus projections the projection axis with the greatest probability of clear projection should be chosen.

Finally, modulus projections have the advantage that 'heavy atom' derivatives of complex organic molecules can be solved *ab initio* with partial three-dimensional data, thus placing analysis within the scope of laboratories not equipped with automatic computers for handling the complete three-dimensional data otherwise necessary for these compounds.

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A New Method for Calculating the Effect of the Collimating System on the Small-Angle X-ray Scattering Pattern

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The angular distribution of small-angle X-ray scattering, corrected for the effects of the collimating system, is expressed in terms of the pair distribution function. This formulation, which has not previously been used for determination of collimation corrections, is convenient when the slit height or scattering angle is large. When the slits are of infinite height and negligible width, the slit-corrected functions are almost as easy to calculate as the perfect-collimation functions. Evaluation in terms of known functions is made for hollow spheres of uniform charge density, and the results are tabulated. The use of the tables for analysis of scattering data is described.

1. Introduction

In recent years the scattering of X-rays at angles of 5° or less has been used to gain information about the size and shape of particles in the size range 20–2000 Å, including several viruses and proteins (Ritland, Kaesberg & Beeman, 1950; Leonard, Anderegg, Shulman, Kaesberg & Beeman, 1953; Schmidt, Kaesberg & Beeman, 1954). Under these conditions the small-angle scattering is due to diffraction from small particles and is little affected by atomic structure.

A common practice in the analysis of the scattering data is to compare the experimental scattering curves with scattering curves calculated under the assumption of a dilute solution of identical particles of a particular shape. This procedure is in practice usually preferable to an inversion of the scattering curve, because there may be sufficient uncertainty in the data to make the inverted curve unreliable and because of the difficulty of relating the inverted curve unambiguously to the particle size and shape.

Theoretical scattering patterns have been calculated for a few simple shapes, assuming perfect collimation (Fournet & Guinier, 1950; Porod, 1948–9). However, with collimating slits of the size usually needed to obtain sufficient scattered intensity, the effects of the

slit system on the scattering pattern are appreciable. The correction of calculated scattering patterns for imperfect collimation is reviewed by Kratky, Porod & Kahovec (1951) and by Anderegg (1952), who derived a general expression for the slit-corrected scattering pattern. However, his result is difficult to apply for large slit heights and for the relatively large scattering angles at which data have now been obtained (Leonard *et al.*, 1953; Schmidt *et al.*, 1954).

In this paper a new method is presented for calculating scattering patterns for arbitrary slit dimensions. The result is expressed in terms of the pair distribution function, which previously was used only with perfect collimation. For slits of infinite height and negligible width the expression takes a particularly simple form. In many experimental situations the collimation is nearer to that of slits of infinite height and negligible width than to that of perfect collimation. Scattering patterns calculated for collimation by slits of infinite height and negligible width should therefore be useful. Tables of these slit-corrected functions, obtained by the author's method, are given for hollow spheres of uniform charge density.

2. Evaluation of the scattering function

According to the Debye scattering formula (Compton & Allison, 1935), the angular distribution $I(k)$ of scattered X-ray intensity from a rigid array of N point charges which can rotate freely as a unit is given by

$$I(k) = \frac{1}{N^2} \sum_{i=1}^{N} \sum_{j=1}^{N} \frac{\sin kr_{ij}}{kr_{ij}} ,$$

where

$$k = 4\pi \sin \tfrac{1}{2}\varphi/\lambda$$

and where r_{ij} is the distance between charges i and j, φ is the scattering angle, and λ is the wavelength. The values of $I(k)$ are normalized so that $I(0) = 1$.

For an extended charge distribution $\varrho(\mathbf{r})$ the analogue of the Debye formula is obtained by replacing the double summations by two volume integrations. If for one volume integration a spherical coordinate system u, φ, θ is used with origin at a point $\mathbf{r}_1$ in the other volume integration and with $\mathbf{r}_1$ as z axis, then u corresponds to r_{ij} in the Debye formula. When the order of integration is chosen so that the integration over u is performed last, the scattered intensity $I(k)$ can be written

$$I(k) = \int_0^\infty du H(u) \frac{\sin ku}{k} , \qquad (1)$$

where

$$H(u) = u \int \sin\theta d\theta \int d\varphi \int_{V_1} dV_1 \varrho(\mathbf{r}_1)\varrho(\mathbf{r}_1+\mathbf{u}) .$$

The V_1 integration is over the coordinates $\mathbf{r}_1$. A point in the spherical coordinate system is denoted by $\mathbf{u}$, and the charge density is normalized so that

$$\int_V \varrho(\mathbf{r}) dV = 1 .$$

This formulation of $I(k)$ is discussed by Porod (1948–9). The probability of finding charged regions a distance u apart is given by $uH(u)$. Often $uH(u)$ is referred to as the pair distribution function and is called the distance function by Porod.

If the volume integration is assumed to extend through all space, as can be done without loss of generality if $\varrho(\mathbf{r})$ is taken to be zero for regions containing no charge, then, for a spherical charge distribution $(1/4\pi)\varrho(r)$,

$$H(u) = \frac{u}{2} \int_0^\infty dr_1 r_1^2 \varrho(r_1) \int_0^\pi d\theta \sin\theta \varrho(T) ,$$

where

$$T = [r_1^2+u^2-2r_1 u \cos\theta]^{\frac{1}{2}} .$$

Let

$$s = T+r_1, \quad t = T-r_1 .$$

Then $H(u)$ can be expressed as an integral over s and t, giving

$$H(u) = \tfrac{1}{4} \int_u^\infty ds \int_{-u}^{u} \bar{\varrho}(s,t) dt , \qquad (2)$$

where

$$\bar{\varrho}(s,t) = \tfrac{1}{4}(s^2-t^2) \varrho\left(\frac{s-t}{2}\right) \varrho\left(\frac{s+t}{2}\right) .$$

The slit-corrected scattering function $P(k)$ has been shown (Anderegg, 1952; Kratky *et al.*, 1951) to be related to the perfect collimation function $I(k)$ by the equation

$$P(k) = A \int_0^\infty d\beta W_h(\beta) \int_{-\infty}^{\infty} W_w(\alpha) I(g) d\alpha ,$$

where A is a normalization constant usually chosen to make $P(0)$ equal to unity, $W_h(\beta)$ and $W_w(\alpha)$ are weighting functions for the slit heights and widths, respectively, and

$$g = (4\pi/\lambda) \sin \tfrac{1}{2}[(\varphi-\alpha)^2+\beta^2]^{\frac{1}{2}} .$$

The calculation of the weighting functions, which depend on the type of collimation used, is described by Anderegg (1952). If one defines the function

$$G(k,u) = A \int_0^\infty d\beta W_h(\beta) \int_{-\infty}^{\infty} d\alpha W_w(\alpha) \frac{\sin gu}{g} ,$$

then $P(k)$ can be put in the form

$$P(k) = \int_0^\infty H(u) G(k,u) du . \qquad (3)$$

It can be seen that $P(k)$ is the integral of the product of two functions, one depending on the type of collimation and the other on the particle shape. In calculating the effects of the slit system, only $G(k,u)$ must be considered, while the shape of the scattering particle affects only $H(u)$. Therefore the effect of the collimating system on the perfect collimation functions is seen to be the replacement of $K^{-1} \sin ku$ in (1) by $G(k,u)$.

By a Fourier inversion, using (1), $H(u)$ can be calculated from $I(k)$. An analogous inversion can in

principle be performed with (3). Alternatively the inversion of (3) can be broken up into two steps. The perfect collimation function $I(k)$ is first found by operating on the slit-corrected function and a Fourier inversion is then used to find $H(u)$. Methods for obtaining the perfect collimation function from the slit-corrected function are described by Anderegg (1952), and by Kratky *et al.* (1951).

For slits of infinite height and negligible width, $W_w(\alpha)$ is the delta function $\delta(\alpha)$, and $W_h(\beta)$ is constant over all angles for which $I(k)$ is appreciable. Assuming the wavelength is small enough that the angular extent of the scattering pattern is so small that $\sin\frac{1}{2}\varphi$ can be replaced by $\frac{1}{2}\varphi$, gives the result obtained by Guinier & Fournet (1947):

$$P(k) = \int_0^\infty d\beta_1 I(x) \Big/ \int_0^\infty d\beta_1 I(\beta_1) , \tag{4}$$

where

$$x = [k^2+\beta_1^2]^{\frac{1}{2}} \quad \text{and} \quad \beta_1 = 2\pi\beta/\lambda .$$

Using (1),

$$P(k) = \int_0^\infty du H(u) J_0(ku) \Big/ \int_0^\infty du H(u) . \tag{5}$$

Thus when the slits are of infinite height and negligible width, $G(k, u)$ reduces to $J_0(ku)$, and the evaluation of the slit-corrected function is not much more difficult than finding the perfect collimation function.

3. Scattering functions for hollow spheres

For hollow spheres with inner radius ha and outer radius a, and with uniform charge density we have

$$\begin{aligned} &\varrho(r) = 0, \quad 0 \leqslant r < ha; \\ &\varrho(r) = 3/\{a^3(1-h^3)\}, \quad ha \leqslant r \leqslant a; \\ &\varrho(r) = 0, \quad a < r . \end{aligned}$$

When this density function is used to calculate $H(u)$ and the result substituted into (5), the scattering function $P_h(ka)$ for hollow spheres of uniform charge density for slits of infinite height and negligible width is found to be

$$\begin{aligned} P_h(ka) = M(h)[&P_0(ka)+h^5 P_0(kha) \\ &-2N(h, ka)+2N(-h, ka)] , \end{aligned} \tag{6}$$

where

$$\left.\begin{aligned} M(h) &= (1-\tfrac{5}{2}h^3+\tfrac{3}{2}h^5)^{-1} , \\ N(h, ka) &= \left(\frac{1+h}{2}\right)^5 P_0\left(\frac{1+h}{2}ka\right) \\ &\quad -5\left(\frac{1-h}{2}\right)^2\left(\frac{1+h}{2}\right)^3 P_2\left(\frac{1+h}{2}ka\right) , \\ P_0\left(\frac{u}{2}\right) &= \frac{15}{u^5}[(u^2+3)\overline{J}_0(u)+3u^2 J_0'(u)-3uJ_0(u)] , \\ P_2\left(\frac{u}{2}\right) &= \frac{3}{u^3}[(u^2-1)\overline{J}_0(u)+u^2 J_0'(u)+uJ_0(u)] , \\ \overline{J}_0(u) &= \int_0^u J_0(t)\,dt . \end{aligned}\right\} \tag{7}$$

When h is zero, the spheres are solid, and $P_h(ka)$ reduces to $P_0(ka)$, as given by (7). The scattering function for spherical shells of negligible thickness is found from the limit of $P_h(ka)$ as h approaches 1, giving

$$P_1(ka) = \frac{\overline{J}_0(2ka)}{2ka} .$$

4. Series expansions

Expanding (5) in powers of k, we have

$$P(k) = \sum_{n=0}^{\infty} \frac{(-1)^n k^{2n} \int_0^\infty u^{2n} H(u)\,du}{2^{2n}(n!)^2 \int_0^\infty H(u)\,du} . \tag{8}$$

An analogous expansion is possible for (3). The series expansion of (6) is

$$P_h(ka) = \sum_{n=0}^{\infty} c_n F_n(h)(ka)^{2n} , \tag{9}$$

where $M(h)$ is as in (7), and

$$\begin{aligned} c_n &= \frac{30(-1)^n}{(n!)^2(2n+2)(2n+3)(2n+5)} , \\ F_n(h) &= M(h)[1+h^{2n+5}-2Q_n(h)+2Q_n(-h)] , \\ Q_n(h) &= \left(\frac{1+h}{2}\right)^{2n+3}\left[\left(\frac{1+h}{2}\right)^2 - \frac{2n+5}{2n+1}\left(\frac{1-h}{2}\right)^2\right] . \end{aligned}$$

For uniform spheres h is zero, and

$$P_0(ka) = \sum_{n=0}^{\infty} c_n (ka)^{2n} . \tag{10}$$

For spherical shells of negligible thickness, h approaches 1, and the resulting limit of (9) is

$$P_1(ka) = \sum_{n=0}^{\infty} \frac{(-1)^n (ka)^{2n}}{(n!)^2(2n+1)} .$$

A series expansion can be obtained for the angular distribution of scattering, $P(v, ka)$, for ellipsoids of revolution of uniform charge density and with semi-major axis va and equatorial radius a, corrected for the effects of slits of infinite height and negligible width. If the perfect collimation scattering function derived by Guinier (1939) is substituted into (4), a change of variables and order of integration gives

$$P(v, ka) = (\cosh^{-1} v)^{-1} \int_1^v dy (y^2-1)^{-\frac{1}{2}} P_0(kay) , \quad v > 1 ,$$

$$P(v, ka) = (\cos^{-1} v)^{-1} \int_v^1 dy (1-y^2)^{-\frac{1}{2}} P_0(kay), \quad v < 1 ,$$

where $P_0(ka)$, given by (7), is the uniform-sphere scattering function corrected for slits of infinite height and negligible width. Using (10), we have

$$P(v, ka)\sum_{n=0}^{\infty} = c_n f_n(v)(ka)^{2n}, \qquad (11)$$

where $f_0(v) = 1$ for all v, and for $n > 0$,

$$\left.\begin{aligned} f_n(v) &= [(2n+1)b_n]^{-1}[1+B(v)\sum_{j=0}^{n=1} b_j v^{2j+1}], \\ b_j &= 2^{2j}(j!)^2/(2j+1)!, \\ B(v) &= (v^2-1)^{\frac{1}{2}}(\cosh^{-1} v)^{-1}, \qquad v \geqslant 1, \\ B(v) &= (1-v^2)^{\frac{1}{2}}(\cos^{-1} v)^{-1}, \qquad v \leqslant 1. \end{aligned}\right\} \qquad (12)$$

Tables of (11) are available from the author.

5. Numerical calculations

A desk computer and an IBM 602-A calculating punch were used to obtain the results given in the tables. The error should be no greater than one unit in the last figure shown.

The slit-corrected scattering function $P_h(ka)$ was evaluated for $0 \leqslant 2ka \leqslant 40$, with $2ka$ varying in steps of 0·2, for h values of 0·0, 0·3, 0·6, 0·8, 0·9, and 1·0. A summary of these results is given in Table 1, which lists $P_h(ka)$, for all the above h values, with $2ka$ running in steps of 1 from 2 to 40. Complete tables, with second differences, are available from the author.

For the calculation of the tables of $P_h(ka)$, tables of $\overline{J}_0(x)$ are needed. The tables of Lowan & Abramowitz (1943) were used for the interval $0 \leqslant x \leqslant 10$. For $10 \leqslant x \leqslant 40$, $\overline{J}_0(x)$ had to be calculated. Tables of $\overline{J}_0(x)$ for $10 \leqslant x \leqslant 40$ are being published in another journal (Schmidt, 1955).

Table 1. *Values of* $P_h(ka)$

	$P_h(ka)$					
$2ka$	$h = 0·0$	$h = 0·3$	$h = 0·6$	$h = 0·8$	$h = 0·9$	$h = 1·0$
1	0·94765	0·94638	0·93950	0·93109	0·92577	0·91973
2	0·80454	0·80007	0·77653	0·74877	0·73173	0·71289
3	0·60720	0·59921	0·55898	0·51479	0·4893	0·46252
4	0·40145	0·39143	0·34486	0·30018	0·2775	0·25618
5	0·22685	0·21749	0·18052	0·15522	0·1470	0·14306
6	0·10554	0·099597	0·086171	0·09247	0·1030	0·11770
7	0·039294	0·038506	0·054220	0·08977	0·1130	0·13638
8	0·014626	0·019105	0·059126	0·10887	0·1327	0·15134
9	0·012198	0·020532	0·072485	0·11767	0·1324	0·13914
10	0·015636	0·025551	0·075443	0·10396	0·1080	0·10670
11	0·016202	0·025433	0·063401	0·075263	0·07525	0·076345
12	0·012575	0·019550	0·042758	0·047896	0·05303	0·064510
13	0·0074683	0·011595	0·023431	0·034084	0·04919	0·070340
14	0·0038323	0·005376	0·012105	0·034976	0·05743	0·080048
15	0·0027056	0·002435	0·009457	0·042439	0·06468	0·080344
16	0·0032057	0·002010	0·011626	0·046415	0·06188	0·068804
17	0·0038012	0·002422	0·013790	0·041912	0·04970	0·053680
18	0·0035675	0·002489	0·013161	0·031157	0·03612	0·045184
19	0·0025986	0·002050	0·009849	0·020494	0·02913	0·046681
20	0·0015764	0·001587	0·005746	0·015180	0·03066	0·052919
21	0·0010664	0·001529	0·002731	0·015973	0·03605	0·055667
22	0·0011189	0·001845	0·001498	0·019474	0·03861	0·051018
23	0·0013719	0·002154	0·001538	0·021256	0·03501	0·042069
24	0·0014346	0·002101	0·001881	0·019098	0·02731	0·035357
25	0·0011901	0·001650	0·001874	0·014082	0·02063	0·034841
26	0·00081110	0·001064	0·001460	0·009196	0·01869	0·038810
27	0·00054911	0·0006608	0·0009546	0·006872	0·02115	0·041990
28	0·00051488	0·0005699	0·0006470	0·007384	0·02438	0·040464
29	0·00062125	0·0006827	0·0005864	0·009057	0·02466	0·034897
30	0·00069560	0·0007845	0·0006349	0·009802	0·02115	0·029475
31	0·00063557	0·0007361	0·0006555	0·008654	0·01615	0·027918
32	0·00047552	0·0005570	0·0006288	0·006223	0·01292	0·030285
33	0·00032971	0·0003684	0·0006214	0·003958	0·01302	0·033260
34	0·00028259	0·0002730	0·0006783	0·002952	0·01523	0·033346
35	0·00032503	0·0002799	0·0007624	0·003242	0·01687	0·029931
36	0·00037892	0·0003209	0·0007928	0·003990	0·01605	0·025574
37	0·00037372	0·0003284	0·0007337	0·004246	0·01307	0·023493
38	0·00030297	0·0002914	0·0006356	0·003643	0·009947	0·024681
39	0·00021811	0·0002530	0·0005924	0·002526	0·008638	0·027209
40	0·00017560	0·0002573	0·0006545	0·001554	0·009475	0·028144

Table 2. *Maxima and minima of* $P_h(ka)$

h	$(2ka)$	$P_h(ka)$	h	$(2ka)$	$P_h(ka)$	h	$(2ka)$	$P_h(ka)$
0·0	8·6506	0·011 680	0·6	7·2575	0·053 167	0·9	8·493	0·135 9
0·0	10·624	0·016 541	0·6	9·6964	0·076 189	0·9	12·71	0·048 56
0·0	15·037	0·002 7045	0·6	14·882	0·009 421	0·9	15·26	0·065 08
0·0	17·256	0·003 8332	0·6	17·306	0·013 941	0·9	19·28	0·028 80
0·0	21·350	0·001 0339	0·6	22·400	0·001 416	0·9	21·94	0·038 63
0·0	23·704	0·001 4494	0·6	24·490	0·001 938	0·9	25·86	0·018 64
0·0	27·641	0·000 50296	0·6	28·819	0·000 5842	0·9	28·58	0·025 04
0·0	30·086	0·000 69615	0·6	30·820	0·000 6565	0·9	32·45	0·012 57
0·0	33·928	0·000 28233	0·6	32·658	0·000 6174	0·9	35·20	0·016 93
0·0	36·436	0·000 38602	0·6	35·841	0·000 7941	0·9	39·05	0·008 635
			0·6	38·928	0·000 5921			
0·3	8·3237	0·018 262				1·0	5·8843	0·117 38
0·3	10·483	0·026 329	0·8	6·5241	0·085 89	1·0	8·0839	0·151 45
0·3	15·736	0·001 972	0·8	8·9052	0·117 78	1·0	12·076	0·064 458
0·3	17·612	0·002 536	0·8	13·398	0·032 989	1·0	14·530	0·081 839
0·3	20·616	0·001 494	0·8	15·994	0·046 415	1·0	18·313	0·044 683
0·3	23·388	0·002 187	0·8	20·322	0·014 871	1·0	20·887	0·055 718
0·3	27·808	0·000 5655	0·8	22·976	0·021 257	1·0	24·567	0·034 284
0·3	30·219	0·000 7887	0·8	27·263	0·006 775	1·0	27·214	0·042 113
0·3	34·380	0·000 2661	0·8	29·912	0·009 810	1·0	30·829	0·027 854
0·3	36·652	0·000 3317	0·8	34·206	0·002 925	1·0	33·528	0·033 792
0·3	39·411	0·000 2483	0·8	36·807	0·004 263	1·0	37·097	0·023 476
			0·9	6·190	0·102 1	1·0	39·833	0·028 188

In Table 2 are given the maxima and minima of Table 1, with the values of $P_h(ka)$ at the maxima and minima. The location of the maxima and minima were taken from roots of the derivative of Everett's interpolation formula, using second differences. The interpolation formula was then used to evaluate the function at the maxima and minima.

By direct numerical integration of (4), $P_h(ka)$ for $h = 0$ has been calculated previously by Anderegg (1952). His results, which also include locations of maxima and minima, agree with Tables 1 and 2 within about 1%.

6. Applications

Although the infinite-slit-height approximation is not always valid, there are many cases when the infinite-slit-height functions are more nearly applicable than the perfect-collimation functions. Therefore Tables 1 and 2 will often be useful for analysis of data when the slit height is much larger than the slit width.

If a scattering particle is believed to be spherical, from evidence such as electron micrographs or X-ray scattering patterns with secondary maxima and minima, an attempt can be made to fit the data with calculated scattering patterns for spheres. The curve for uniform spheres ($h = 0$) should ordinarily be tried first, as it is the simplest case. If a satisfactory fit cannot be obtained, the hollow-sphere functions can then be used.

In fitting theoretical scattering curves to experimental data, two general features of the curves must be considered. The locations of the secondary maxima and minima of the calculated curve must coincide with those of the data, and also the intensities of the secondary maxima and minima must agree. By the use of the following equation the radius a of the sphere can be determined from the location of the experimental angles φ/m at which maxima and minima occur:

$$(ka)_m = 4\pi a\lambda^{-1} \sin \tfrac{1}{2}\varphi_m .$$

The X-ray wavelength is λ, and $(ka)_m$ is the argument of the theoretical scattering function at which the maximum or minimum corresponding to φ_m occurs. The assumption of particle shape is considered verified if the radius values obtained from different maxima and minima agree within experimental error.

The values of $(ka)_m$ depend on h. If one plots $\log (ka)_m$ as ordinate and h as abscissa, with the curves for all maxima and minima on the same axes, an estimate of $(ka)_m$ can be made for h values not listed in Table 2. Moreover, if a plot of $\log \varphi_m$ is made on the y axis of another piece of the same type of graph paper, the logarithmic ordinates enable the point of best fit of locations of maxima and minima to be determined merely by moving one paper relative to the other. An estimate of both h and a can be found by this process. However, since the curves of $\log (ka)_m$ are nearly parallel for $0{\cdot}6 \leqslant h \leqslant 1{\cdot}0$ for the first three maxima and minima, a unique choice of radius and h is sometimes not possible without data at larger scattering angles or without consideration of scattered intensities.

The results from the location of maxima and minima can be checked by comparison of the experimental and theoretical intensities at the maxima and minima. However, the agreement may not be as good as found from the location of maxima and minima, since the intensities are more sensitive to deviations from the assumed collimation conditions than are the locations of the maxima and minima.

A new analysis of the scattering data for the protein particle associated with turnip yellow mosaic virus (Schmidt *et al.*, 1954) has been made using the methods outlined above. At the time the data were published, hollow-sphere functions corrected for slits of infinite height and negligible width had not been calculated, and so the data were interpreted by extrapolation from available calculations, giving a sphere radius of 140 Å, and an h of 0·75. Applying the same correction for the effects of the finite slit widths as was used by Schmidt *et al.* for turnip yellow mosaic nucleoprotein, use of Tables 1 and 2 and the methods described above essentially confirms the previous results.

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The Splitting of Layer Lines in X-ray Fibre Diagrams of Helical Structures: Application to Tobacco Mosaic Virus

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The layer lines in X-ray fibre diagrams of tobacco mosaic virus gel have been observed to be split, the extent of the splitting varying with the strain of the virus. This effect is interpreted in terms of the helical arrangement of the protein sub-units about the long axis of the particle, and has stimulated some general remarks on diffraction by structures of this type.

Introduction

X-ray fibre diagrams of highly orientated preparations of tobacco mosaic virus (TMV) were first obtained by Bernal & Fankuchen (1941). Watson (1954) observed that the diagrams contained prominent features characteristic of helical structures, and suggested that the virus particle, of diameter 150 Å and length 3000 Å (Williams & Steere, 1951) was in fact one giant helical molecule, identical protein units being set in helical array around the long axis. He showed that in the axial repeat period of 69 Å there were $3n+1$ such protein units distributed over 3 turns of the helix. It is not possible to determine unequivocally, from high-angle meridional reflexions, whether n is 10 (Watson, 1954) or 12 (Franklin, 1955), but a recent interpretation (to be published) of certain other features of the X-ray diagram favours the value 10, giving 31 protein units in 3 turns of the helix.

We have now observed that in fibre diagrams of TMV the intensity maxima do not lie *exactly* on a set of equally spaced layer lines. If one chooses the set of equally spaced layer lines which gives the best fit with the diagram as a whole, then one finds that the layer lines whose order is a multiple of 3 ($l = 3n$) have maxima lying exactly on them, whereas for the layer lines $l = 3n+1$ and $l = 3n+2$ the maxima are displaced to a small distance on either side of the mean layer-line position. The extent of the effect varies with the strain of the virus. This phenomenon is readily explained in terms of the suggested helical arrangement of the protein units of which the virus particle