

## The Diffraction of X-rays by a Cylindrical Lattice. I

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The diffraction of X-rays by a cylindrical lattice is of interest in connection with the structure of chrysotile and some other minerals. A cylindrical lattice model is defined, and it is shown to give a set of reflexions in the same directions as certain of the reflexions from a rotating crystal. These reflexions have a shape similar to that of reflexions from a normal crystal, and their integral breadth is evaluated in terms of the number of co-operating cylindrical layers. The amplitudes of the reflexions are related to the Fourier coefficients of the electron-density distribution projected on to a radial plane, provided that the projection is defined in a special way. A second set of reflexions is also produced which is analogous to, but not identical with, that from a cross-grating.

### 1. Introduction

It has been shown by electron microscopy that the ultimate particles of the silicate minerals chrysotile, garnierite, and halloysite, have the form of hollow cylinders (Bates, Sand & Mink, 1950; Noll & Kircher, 1951, 1952). Of these minerals chrysotile has been studied extensively by X-ray diffraction, and it has been known for many years that oriented fibres of chrysotile give diffraction patterns which resemble in some respects those given by rotating single crystals (Warren & Bragg, 1930; Aruja, 1943). These workers, and more recently Padurow (1950) and Whittaker (1951, 1952) have discussed the form and dimensions of the unit cell of chrysotile on the assumption that, in so far as the diffraction pattern appears to resemble a single-crystal rotation photograph, it may be treated as such. Structure analyses of chrysotile of varying degrees of completeness (Warren & Hering, 1941; Aruja, 1943; Whittaker, 1953) have also been made on the same assumption, and have shown that starting from this assumption it is possible to interpret the diffraction pattern on the basis of a layer structure corresponding to a magnesium analogue of the kaolin minerals. It has been pointed out by Pauling (1930) that the layers in such a structure would be expected to curve, and Whittaker (1953) has adduced evidence, from the detailed structure analysis, that this is indeed the case. It follows that the tubular form observed by electron microscopy is no mere habit phenomenon, but corresponds to the existence of a tubular layer structure. This at once suggests the possibility of a self-contradiction within the published structural work, since this has been carried out as though the diffraction pattern were that of a normal rotating single crystal, or an assembly of such normal crystals oriented with one axis parallel. The present work is therefore devoted to a theoretical analysis of the diffraction from a tubular structure of this type, in order to ascertain the extent to which it resembles, and the

extent to which it differs from, the diffraction from a normal rotating crystal.

It seems physically probable that a cylindrically curved layer structure would adopt a spiral form rather than the form of a set of coaxial circular cylinders, although it may be noted that the relationship

$$nb = 2\pi a',$$

where  $a'$  is the interlayer spacing,  $b$  is the circumferential repeat distance and  $n$  is an integer, is (at least approximately) obeyed by chrysotile, with a value of  $n = 5$ . The latter form cannot, therefore, be ruled out. Moreover, the theory of diffraction by such a spiral cylinder involves mathematical difficulties which are still under investigation, and it may be supposed that the two cases will not differ excessively from one another. The theory presented is therefore that for a set of layers in the form of coaxial circular cylinders.

Some of the characteristics of diffraction by cylindrical structures have been discussed by Oster & Riley (1952), but their results are not sufficiently general for the present purpose. Other results have been obtained by Fock & Kolpinsky (1940) and by Blackman (1950), and these will be referred to later.

### 2. Nomenclature and assumptions

If we consider a set of congruent plane lattices wrapped into the form of a set of coaxial circular cylinders with their radii in arithmetic progression, then it follows that there must be complete azimuthal disorder between successive cylinders, because the same arcual repeat distances on different cylinders will subtend different angles at the axis. Therefore, in order to simplify the problem, we consider a lattice in which the diffracting matter is distributed uniformly in azimuth. The effect of this assumption is considered in § 7. The further definition of the distribution of

diffracting matter is most conveniently made in terms of the following coordinate system.

Let the  $z$  axis lie along the common axis of the cylinders, and let an arbitrary origin  $O$  be taken on the  $z$  axis. Then let the position of any point  $A$  be defined in terms of the coordinates  $\rho, \varphi, z$ , where

$\rho$  is the distance of  $A$  from the  $z$  axis, measured parallel to the surface of a cone of a semi-vertical angle  $\pi - \beta$ , coaxial with the cylinders, and with its vertex at  $O$ ;

$z$  is the distance of  $A$  from the surface of this cone measured parallel to the  $z$  axis; and

$\varphi$  is the dihedral angle between the plane  $\rho Oz$  and an arbitrary initial radial plane.

Then if  $G(\rho, \varphi, z)$  is the density of diffracting matter at the point  $\rho, \varphi, z$  we define the lattice as a distribution of diffracting matter such that

$G(\rho, \varphi, z) \sin \beta d\rho dz = g$  when  $\rho = a_0 + ma$  and  $z = nc$   
and

$$G(\rho, \varphi, z) = 0 \text{ elsewhere,} \quad (1)$$

where  $g, a_0, a$  and  $c$  are constants, and  $m, n$  may take a range of integral values.

The diffracting matter is thus distributed with a uniform linear density  $g$  along circles which lie at the loci of intersection of a set of coaxial cylinders of radii  $(a_0 + ma) \sin \beta$  and a set of cones, coaxial with the cylinders, with semi-vertical angle  $\pi - \beta$ , and displaced by successive steps, equal to  $c$ , parallel to their common axis. This distribution provides a lattice model, corresponding to clino-chrysotile, but in which the distribution of matter round the cylinders is smoothed to a mean value. If  $\beta$  is put equal to  $\frac{1}{2}\pi$  we obtain a lattice model corresponding in the same way to ortho-chrysotile.

### 3. The reflexion conditions for the cylindrical lattice

In accordance with the usual theory of diffraction, the amplitude of a diffracted ray at a distant point, distant  $R$  from the origin, is given by

$$F(\mathbf{S}) = \frac{Q}{R} \int_{\mathbf{r}} G(\mathbf{r}) \exp\left(\frac{2\pi i}{\lambda} \mathbf{r} \cdot \mathbf{S}\right) dv, \quad (2)$$

where

$Q$  is the electron-scattering function,

$\mathbf{r}$  is the position vector of the point  $\rho, \varphi, z$ ,

$\mathbf{S}$  is the diffraction vector,

and

$\lambda$  is the wavelength.

We then express  $\mathbf{r}$  in terms of  $\rho, \varphi, z$ , and  $\mathbf{S}$  in terms of a set of coordinates  $\rho^*, \gamma, z^*$ , reciprocal to these, which we define as follows:

$\rho^*$  is the distance of a point in diffraction space measured outward from the convex surface of a cone with vertex  $O$  and semi-vertical angle  $\frac{1}{2}\pi - \beta$  and with its axis along the  $z$  axis. The distance  $\rho^*$  is measured parallel to the plane through  $O$  perpendicular to the  $z$  axis.

$z^*$  is the distance of a point in diffraction space from this plane, measured in a direction parallel to the above conical surface.

$\gamma$  is the dihedral angle between  $\rho^* Oz^*$  and the initial plane in terms of which  $\varphi$  was defined.

In terms of these variables (2) becomes

$$F(\rho^*, \gamma, z^*) = \frac{Q}{R} \iiint G(\rho, \varphi, z) \times \exp\left\{\frac{2\pi i}{\lambda} [\rho(\rho^* - z^* \cos \beta) \sin \beta \cos(\varphi - \gamma) + \rho z^* \sin \beta \cos \beta + z z^* \sin \beta]\right\} \rho \sin^2 \beta d\rho d\varphi dz, \quad (3)$$

where the integrations are to extend over the whole volume of the fibre.

Inserting the conditions on  $G(\rho, \varphi, z)$  given in (1), we can reduce two of the integrals in (3) to summations. We are also able to effect a partial separation of the variables, and to obtain an integral which can be evaluated directly as follows:

$$F(\rho^*, \gamma, z^*) = \frac{Qg}{R} \sum_n \exp\left[\frac{2\pi i}{\lambda} ncz^* \sin \beta\right] \times \sum_m \exp\left[\frac{2\pi i}{\lambda} (a_0 + ma)z^* \sin \beta \cos \beta\right] \times \int_0^{2\pi} (a_0 + ma) \sin \beta \exp\left[\frac{2\pi i}{\lambda} (a_0 + ma) \times (\rho^* - z^* \cos \beta) \sin \beta \cos(\varphi - \gamma)\right] d\varphi \quad (4)$$

$$= \frac{Qg}{R} \sum_n \exp\left[\frac{2\pi i}{\lambda} ncz^* \sin \beta\right] \times \sum_m \exp\left[\frac{2\pi i}{\lambda} (a_0 + ma)z^* \sin \beta \cos \beta\right] \times 2\pi(a_0 + ma) \sin \beta J_0\left[\frac{2\pi}{\lambda} (a_0 + ma)(\rho^* - z^* \cos \beta) \sin \beta\right]. \quad (5)$$

The first summation in (5) is exactly the same as that which occurs in the theory of diffraction by a normal crystal. It has appreciable values only in the vicinity of the planes in reciprocal space

$$z^* = l\lambda/c \sin \beta, \quad \text{where } l \text{ is an integer.}$$

It follows that the rays diffracted from our model fibre will give rise on a photograph to layer lines of the usual form.

The second summation in (5) defines the distribution of the diffracted amplitude on any such layer plane. The summation is independent of  $\gamma$ , and therefore has

circular symmetry. Its form may be conveniently evaluated if we introduce the approximation

$$J_0(x) \simeq (2/\pi x)^{\frac{1}{2}} \cos(x - \frac{1}{4}\pi).$$

This approximation is valid to within 2% of the value of the nearest maximum of  $J_0(x)$  for most values of  $x$  in which we are interested in practice (for the exception see below), and over the greater part of the range to a much higher degree of accuracy than this. (The range of interest is about  $0.04 < \xi < 2.0$  for Cu  $K\alpha$  radiation. With a probable minimum value of  $a_0 = 4a$  and a maximum value of  $m = 14$ , this gives a range of  $5 < x < 1000$ .) If we introduce this approximation in exponential form into (5), the summation with respect to  $m$  becomes

$$\left(\frac{\lambda \sin \beta}{\xi}\right)^{\frac{1}{2}} \left\{ \sum_m (a_0 + ma)^{\frac{1}{2}} \exp \left[ \frac{2\pi i}{\lambda} \varrho^* \sin \beta (a_0 + ma) - \frac{1}{4}\pi i \right] + \sum_m (a_0 + ma)^{\frac{1}{2}} \exp \left[ \frac{2\pi i}{\lambda} (2z^* \cos \beta - \varrho^*) \times \sin \beta (a_0 + ma) + \frac{1}{4}\pi i \right] \right\}. \quad (6)$$

The first summation in (6) has appreciable values only in the vicinity of

$$\varrho^* = h\lambda/a \sin \beta, \quad \text{where } h \text{ is a positive integer,}$$

and similarly the second summation has appreciable values only where

$$\varrho^* = 2z^* \cos \beta - h\lambda/a \sin \beta, \quad \text{where } h \text{ is a negative integer.}$$

The distribution of intensity in reciprocal space is therefore confined to rings whose positions are approximately specified by

$$\xi = ha^* \pm lc^* \cos \beta, \quad \zeta = lc^* \sin \beta,$$

where  $a^*$  and  $c^*$  are related to  $a$  and  $c$  in the usual way. The intensity of these rings will be inversely proportional to  $\xi$  on account of the factor  $(\lambda \sin \beta/\xi)^{\frac{1}{2}}$  in (6). In a practical diffraction experiment, however, the intensity recorded for each ring (after making allowance for geometrical factors and other experimental corrections) will be that contained within an angular range of  $\mathcal{V}$  equal to  $\delta$ , where  $\delta$  is the divergence of the incident beam. The corrected observed intensities will therefore all be equal and independent of  $\xi$ .

The approximation for the Bessel function in terms of a cosine is not valid for  $\xi \simeq 0$ , i.e. for reflexions with  $h = 0$  when  $\beta = \frac{1}{2}\pi$ . However, since all the Bessel functions in the summation (5) have maxima at  $\xi = 0$  it follows that a diffraction maximum also occurs in this position.

Thus it is concluded that a cylindrical lattice of the type considered gives reflexions in the same directions as the  $h0l$  reflexions from a three-dimensional rectangular lattice rotating about its  $c$  axis and having the same  $a$  and  $c$  parameters. The intensities of the re-

flexions have effectively the same dependence on direction in both cases.

#### 4. The profile and breadth of the reflexions

For purposes of computation it is convenient to use  $h$  as the continuous variable and to normalize the reflexion intensity to have a maximum value of unity. We therefore compute the function

$$I(h) = \frac{\left| \sum_m (a_0/a + m)^{\frac{1}{2}} \exp [2\pi i h (a_0/a + m) - \frac{1}{4}\pi i] \right|^2}{\left( \sum_m (a_0/a + m)^{\frac{1}{2}} \right)^2}. \quad (7)$$

The results for various ranges of  $m$ , and for two values of  $a_0/a$ , are shown in Fig. 1. The values of these

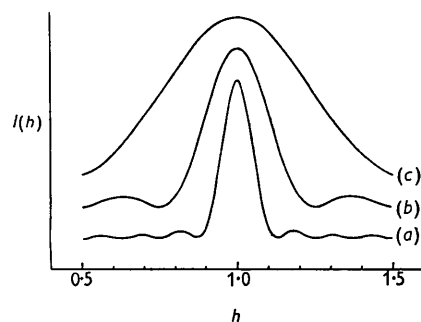


Fig. 1.  $I(h)$  computed from equation (7) with values of  $a_0/a$  and ranges of  $m$  as follows:

(a):	$a_0/a = 8$	$m = 0-7$
(b):	$a_0/a = 8$ or $12$	$m = 0-3$
(c):	$a_0/a = 8$	$m = 0-1$

Successive curves are displaced vertically for clarity.

parameters are chosen within the range which is of interest in the chrysotile problem. The curves exhibit a principal maximum at the integral value of  $h$  together with small subsidiary maxima at either side, and are of a form very similar to those for normal crystal reflexions. The areas under the principal maxima, and hence the integral breadths, have been determined graphically. The integral breadths are found to be

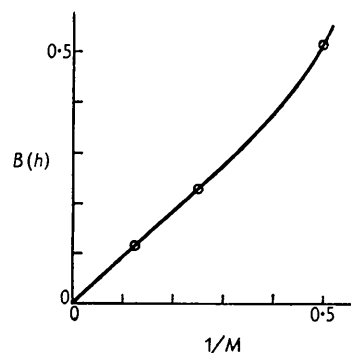


Fig. 2. The integral breadths of the principal maxima as a function of the reciprocal of the number of cooperating cylinders.

independent of the radius of the innermost cylinder, and to vary with the number of cooperating cylinders,  $M$ , as shown in Fig. 2. With  $M > 3$  the relation is found to be

$$B(h) = 0.92/M.$$

This is closely analogous to the corresponding formulae for normal crystals of various shapes.

### 5. The effect of multiplicity on the reflexions

When either  $z^*$  or  $\cos \beta$  becomes zero, expression (6) reduces to

$$2 \left( \frac{\lambda \sin \beta}{\xi} \right)^{\frac{1}{2}} \sum_m (a_0 + ma)^{\frac{1}{2}} \cos \left[ \frac{2\pi}{\lambda} \rho^* \sin \beta (a_0 + ma) - \frac{1}{4}\pi \right]. \quad (8)$$

Expression (8) is proportional to the amplitude of a reflexion of multiplicity 2; i.e. either to a reflexion of the type  $h00 + \bar{h}00$ , or to a reflexion of the type  $h0l + \bar{h}0l$  from a lattice with  $\beta = \frac{1}{2}\pi$  (corresponding to orthochrysolite). It follows that in such circumstances the two reflexions are additive by amplitude, and not by intensity as is the case with multiple reflexions from a single crystal. Physically we may explain the difference as follows. Every reflexion from the cylindrical lattice is being produced continuously and therefore simultaneously. If two such reflexions occur in the same direction they must be capable of mutual interference. Two reflexions in the same direction from a normal rotating crystal always occur consecutively, and their effects are therefore additive by intensity.

The intensity formula corresponding to (8), and analogous to (7), is

$$I(h + \bar{h}) = \frac{4 \left\{ \sum_m (a_0/a + m)^{\frac{1}{2}} \cos [2\pi h (a_0/a + m) - \frac{1}{4}\pi] \right\}^2}{\left( \sum_m (a_0/a + m)^{\frac{1}{2}} \right)^2}. \quad (9)$$

This has a maximum peak value of four times that of (7). However, when  $I(h + \bar{h})$  is plotted and compared with the corresponding curve for  $4I(h)$ , as in Fig. 3,

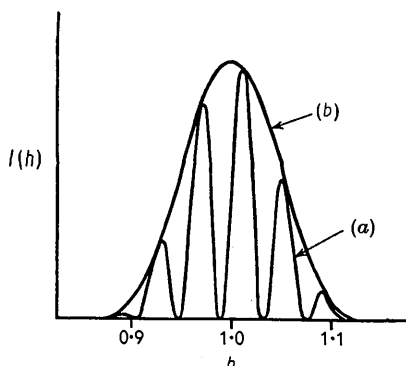


Fig. 3. Comparison of the intensity curve for a multiple reflexion  $h0l + \bar{h}0l$  (curve (a)), with four times that for a single reflexion  $h0l$  (curve (b)). The number of cooperating cylinders is eight in each case.

it is seen that the integrated intensity is only twice that for a single reflexion on account of the fine structure which has appeared. This fine structure arises from the fact that within the single reflexions there exist continuous fluctuations of phase which are disposed differently, in the  $+h$  and  $-h$  reflexions, with respect to the centre of the reflexion. These differences of disposition are such that when the two reflexions are superimposed the phase contrasts are converted to intensity contrasts and the amplitude becomes wholly real, as is shown by expression (8). Thus, in spite of considerable differences in the theory, the effect of multiplicity on the integrated intensity of reflexions from a cylindrical lattice is exactly the same as the corresponding effect for reflexions from a rectilinear lattice.

### 6. The intensity of the reflexions

In a real fibre based on a cylindrical lattice there will exist an electron-density distribution  $G(\rho, \varphi, z)$ . On account of the azimuthal disorder between successive layers of the structure,  $G(\rho, \varphi, z)$  will not be a regularly repeating function in three dimensions, but we may derive from it a regularly repeating function in two dimensions,  $g(\rho, z)$ , in the following way.

Consider a radial plane of the cylinder. From all points of this plane draw circular arcs centred on the cylinder axis and lying in planes perpendicular to that axis. Continue each such arc until a point is reached whose environment *in the cylindrical surface on which it lies* is identical with that at the starting point of the arc. The ends of these arcs will then lie on a serrated surface bounded by sections of radial planes and cylindrical surfaces.† Now sum the electron density along each arc and assign a corresponding weight to the point at its foot on the initial plane. The pattern of weighted points defined in this way will then constitute a regular two-dimensional repeating pattern based on a parallelogram mesh of sides  $a$  and  $c$  and of included angle  $\beta$ . The function  $g(\rho, z)$  which describes this pattern can be defined as

$$g(\rho, z) = \frac{b}{2\pi \rho_m} \int_0^{2\pi} \rho G(\rho, \varphi, z) d\varphi, \quad \rho_m \leq \rho < \rho_{m+1},$$

where  $\rho_m$  is the value of  $\rho$  at the  $m$ th serration. If we also make the approximation (which is examined in § 7)

$$\int_0^\varphi \rho G(\rho, \varphi, z) d\varphi \approx \frac{\varphi}{2\pi} \int_0^{2\pi} \rho G(\rho, \varphi, z) d\varphi, \quad (10)$$

then

$$\rho G(\rho, \varphi, z) d\varphi \approx \frac{\rho_m}{b} g(\rho, z) d\varphi. \quad (11)$$

† The serrations cannot be sharply defined in a real structure unless the electron density is zero at some value of  $\rho$  between the layers. This will be approximately true in any structure which has a sufficiently small steric interaction between successive layers to permit it to adopt a cylindrical layer structure.

Substituting from (11) into (3) and expanding  $g(\rho, z)$  as the double Fourier series

$$g(\rho, z) = \sum_p \sum_q (A_{pq} + iB_{pq}) \exp[-2\pi i(p(\rho - \varepsilon)/a + qz/c)]$$

(where the origin of the plane unit cell is chosen at a distance  $\varepsilon$  from an integral value of  $\rho/a$ ), we obtain, after separating the variables and evaluating the integral with respect to  $\varphi$  as in (5):

$$\begin{aligned} \frac{R}{Q} F(\rho^*, \gamma, z^*) &= \sum_p \sum_q (A_{pq} + iB_{pq}) \\ &\times \int \exp(-2\pi i q z/c) \exp\left(\frac{2\pi i}{\lambda} z z^* \sin \beta\right) dz \\ &\times \sum_m \frac{2\pi \rho_m}{b} \sin^2 \beta \int_{\rho_m}^{\rho_m + 1} \exp\left(-2\pi i p \left(\frac{\rho - \varepsilon}{a}\right)\right) \\ &\times \exp\left(\frac{2\pi i}{\lambda} \rho z^* \sin \beta \cos \beta\right) \\ &\times J_0\left(\frac{2\pi}{\lambda} \rho(\rho^* - z^* \cos \beta) \sin \beta\right) d\rho. \end{aligned} \quad (12)$$

The integral with respect to  $z$  is well known. That with respect to  $\rho$  can be performed with the aid of the readily evaluated integral

$$\int J_0(\alpha x) \exp(-i\alpha x) dx = x \exp(-i\alpha x) (J_0(\alpha x) + iJ_1(\alpha x))$$

provided that

$$\rho^* = p\lambda/a \sin \beta.$$

Hence at the maxima of the reflexions, where  $p = h$  and  $q = l$ , we have

$$\begin{aligned} F(ha^*, \gamma, lc^*) &= (A_{hl} + iB_{hl}) \frac{Q}{R} Nc \frac{2\pi}{b} \sin^2 \beta \exp(2\pi i h \varepsilon/a) \sum_m \rho_m \\ &\times \left[ \rho \exp\left(-2\pi i \left(\frac{h}{a} - \frac{l}{c} \cos \beta\right) \rho\right) \left\{ J_0\left(2\pi \left(\frac{h}{a} - \frac{l}{c} \cos \beta\right) \rho\right) \right. \right. \\ &\left. \left. + iJ_1\left(2\pi \left(\frac{h}{a} - \frac{l}{c} \cos \beta\right) \rho\right) \right\} \right]_{\rho_m}^{\rho_m + 1}. \end{aligned}$$

If we now make the approximation

$$J_0(x) + iJ_1(x) \simeq (2/\pi x)^{\frac{1}{2}} \exp(ix)$$

(which is valid for large  $x$ ) and put

$$\rho_m = a_0 + ma = \mu_m a,$$

we obtain

$$\begin{aligned} F(ha^*, \gamma, lc^*) &= 2(A_{hl} + iB_{hl}) \frac{QNc}{Rb} \left(\frac{\lambda a^3 \sin^2 \beta}{\xi}\right)^{\frac{1}{2}} \exp(2\pi i h \varepsilon/a) \\ &\times \sum_m \mu_m (\mu_{m+1}^{\frac{1}{2}} - \mu_m^{\frac{1}{2}}). \end{aligned} \quad (13)$$

The only quantities in this expression whose moduli vary with the indices of reflexion are  $A_{hl}$ ,  $B_{hl}$  and  $\xi$ .

The presence of the last can be disregarded in practice, as has already been discussed in § 3. It therefore follows that the peak intensity of the reflexion  $h, l$  from a fibre of given size is proportional to  $(A_{hl}^2 + B_{hl}^2)$  only. Since the profiles of the reflexions have been shown to be invariant over the indices, it follows that this proportionality is also true of the integrated intensity.

If the peak function used to define the lattice in § 3 is expressed as a Fourier series, and if the summations  $\sum_m \mu_m (\mu_{m+1}^{\frac{1}{2}} - \mu_m^{\frac{1}{2}})$  in (13) and  $\sum_m \mu_m^{\frac{1}{2}}$ , which occurs at the maxima of the modulus of (5), are approximated by the corresponding integrals, it may be shown that the modulus of (12) is identical with the modulus of (5) at its maxima, within the limits of accuracy of the approximations used.

### 7. The effect of the simplifying assumptions

In defining the cylindrical lattice in § 3 a simplification was effected by letting the diffracting matter be distributed uniformly in azimuth. In § 6 a corresponding assumption was made in using the approximation (10). The effect of this simplification must now be examined.

In the cylindrical lattice let the scattering matter be unchanged in amount but be concentrated at points separated by arcual distances  $b$  along the lattice circles. Let the points nearest to the initial plane and lying on the  $m$ th cylinder have the coordinate

$$\varphi = \delta_m.$$

Then, if  $\nu$  is an integer such that

$$1 \leq \nu \leq 2\pi(a_0 + ma) \sin \beta/b,$$

the density function may be defined by the equation

$$G(\rho, \varphi, z) \rho \sin^2 \beta d\rho d\varphi dz = b g$$

when

$$\rho = a_0 + ma,$$

$$\varphi = \frac{b\nu}{(a_0 + ma) \sin \beta} + \delta_m = \varphi_{m,\nu} \quad (\text{say}),$$

$$z = nc;$$

and the density is zero elsewhere.

The integral with respect to  $\varphi$  in (4) must then be converted into the summation

$$\sum_{\nu} b \exp\left\{\frac{2\pi i}{\lambda} (a_0 + ma) \times (\rho^* - z^* \cos \beta) \sin \beta \cos(\varphi_{m,\nu} - \gamma)\right\}. \quad (14)$$

Following Fock & Kolpinsky (1940), we expand this exponential as a series of Bessel functions to give

$$\sum_{\nu} b J_0 \left[ \frac{2\pi}{\lambda} (a_0 + ma) (\rho^* - z^* \cos \beta) \sin \beta \right] \\ + 2b \sum_{\nu q=1}^{\infty} i^q \cos q(\varphi_{m,\nu} - \gamma) \\ \times J_q \left[ \frac{2\pi}{\lambda} (a_0 + ma) (\rho^* - z^* \cos \beta) \sin \beta \right]. \quad (15)$$

Since  $\nu_{\max} = (2\pi/b)(a_0 + ma) \sin \beta$ , the first sum in (15) is within a negligible error identical with the integral with respect to  $\varphi$  in (4).

Thus the expression for  $F(\rho^*, \gamma, z^*)$  may be split into the sum of two parts: the first part is identical with that examined in § 3, while the second part is

$$2 \frac{Qgb}{R} \sum_n \exp \left[ \frac{2\pi i}{\lambda} ncz^* \sin \beta \right] \\ \times \sum_m \exp \left[ \frac{2\pi i}{\lambda} (a_0 + ma) z^* \sin \beta \cos \beta \right] \\ \times \sum_{\nu q=1}^{\infty} i^q \cos q(\varphi_{m,\nu} - \gamma) \\ \times J_q \left[ \frac{2\pi}{\lambda} (a_0 + ma) (\rho^* - z^* \cos \beta) \sin \beta \right]. \quad (16)$$

The expression (16) clearly has appreciable values only on the layer planes

$$z^* = l\lambda/c \sin \beta.$$

The corresponding diffraction effect on these planes is strictly additive to (6) by amplitude and not by intensity, but following the discussion of multiplicity in § 5 we may conclude that the integrated intensity of the diffraction maxima given by (6) will be additive to the integrated intensity given by (16) over the same region. We may therefore regard (16) as introducing an additional diffraction effect which is superimposed on, but does not modify, that already investigated.

Fock & Kolpinsky (1940) and Blackman (1950) have discussed the diffraction effect from a single layer of a cylindrical lattice as defined above. Their treatment corresponds to consideration of a single term of the summation with respect to  $m$  in (16), and shows that

this corresponds to a series of unsymmetrical reflexions each of which has a sharp head and a long tail extending to higher values of  $\xi$ . Such reflexion profiles resemble qualitatively the cross-grating reflexions given by plane lattices, although they differ quantitatively. The effect of the summation with respect to  $m$  in (16) is to make further quantitative changes in the reflexion profiles compared with those given by Fock & Kolpinsky, and these changes have been studied by numerical computation. The results of these studies, together with further theoretical considerations on the diffuse reflexions will be presented in a subsequent paper.\*

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\* Note added 19 August 1954.—Since the submission of this paper a series of three papers on the diffraction by cylindrical lattices, and its application to the structure of chrysotile, has been published by Jagodzinski & Kunze in *Neues Jahrbuch Monatshefte*. Similar conclusions have been reached independently by these workers.