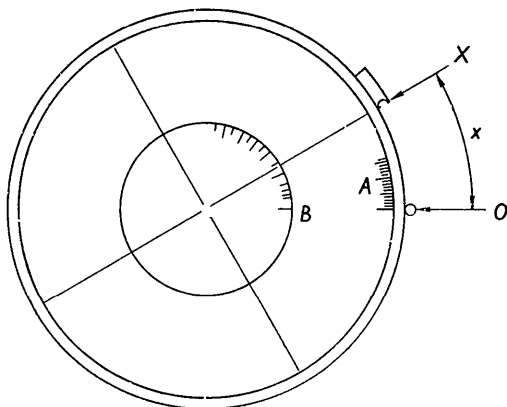


to $2x$, and so on. A simple clutch enables the operator to reverse the direction of motion of the cursor so that $\cos 2\pi(-h)x$ can be obtained from the same angle setting.



The ratchet mechanism for moving the cursor consists of a hardened polished C-shaped steel double pawl pivoted in a recess in the operating and stop-carrying ring, and is sprung with two leaf springs. Either of the directionally opposed pawl faces can be brought into position to engage with the ratchet teeth of the cursor, to transport it in

either direction, by shifting the pressure of the leaf springs on the pawl by means of two knurled knobs which control the spring positions.

The contribution of an atom i to the geometrical structure factor of the form $\cos 2\pi(hx_i \pm lz_i)$ is computed along lines in the reciprocal lattice, say for constant l , by setting the angle stop to x , advancing the cursor to lz_i , and successively determining $\cos 2\pi(hx_i + lz_i)$ from 0 to h , and from 0 to $-h$.

An obvious improvement is the inclusion of a second and third angle stop to hold the values of y and z . If such stops Y and Z are to be added, then X , Y and Z must be capable of being swung out so as not to interfere with one another.

In its present form the device has been found fully accurate and reliable in the summation of $(hx + lz)$. It has been most useful in the (three-dimensional) analysis of phenazine and the (two-dimensional) analysis of tetrabenzonaphthalene (7 and 26 atoms in the asymmetric unit respectively), which are now being carried out in this laboratory. Two hundred F 's of the form $\cos 2\pi(hx_i + lz_i)$ of 26 atoms have been computed in 16 working hours.

It is a pleasure to thank the chief instrument maker of the Weizmann Institute, Mr B. Feldmann, for designing and constructing this instrument.

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An orthorhombic variety of chrysotile. By E. J. W. WHITTAKER, *Research Division, Ferrodo Ltd., Chapel-en-le-Frith, Stockport, England*

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The structure of chrysotile asbestos has been studied by Warren & Bragg (1930), Gruner (1937) and Aruja (1943). Although the detailed structural conclusions of these workers have differed, they have all agreed that the structure is based on a monoclinic cell having the approximate parameters

$$a = 14.6, \quad b = 9.2, \quad c = 5.32 \text{ \AA.}, \quad \beta = 93^\circ 12',$$

or simple multiples or submultiples of these a and b axial lengths.

It appears from the literature that these results were all obtained using specimens from Thetford, Quebec. More recently Padurow (1950) has claimed that the structure is only pseudo-monoclinic and is really triclinic with cell parameters

$$a = 7.36, \quad b = 9.26, \quad c = 5.33 \text{ \AA.}, \\ \alpha = 92^\circ 50', \quad \beta = 93^\circ 11', \quad \gamma = 89^\circ 50'.$$

The chrysotile used in this work was also from Quebec.

As a result of a survey of specimens from a variety of sources in Canada, Rhodesia, Swaziland, India and Australia the author has found that the diffraction patterns obtained differ quite extensively. Certain of these differences have already been reported (Whittaker, 1949), but at the time the nature of the corresponding structural differences had not been ascertained. It has now been found that the photographs may be explained on the assumption that the specimens consist of mixtures, in different proportions, of the normal monoclinic variety

(or pseudo-monoclinic according to Padurow) and a new orthorhombic variety with substantially identical unit-cell dimensions. Chrysotile from Canadian sources does not appear to contain any of the orthorhombic variety, which accounts for this not having been observed by previous workers. The other sources mentioned yield material of varying ortho content both as between sources and as between different specimens from the same source. This content varies from zero up to a value which is still uncertain, but is probably more than 50%. No evidence has been found of fluctuation in this proportion when a specimen is repeatedly halved in cross-section down to a diameter of about 0.05 mm., so that the two varieties are very finely dispersed, quite probably as individual fibrils.

The diffraction phenomena given by ortho-chrysotile closely resemble those given by the clino variety. Similar restrictions exist on the indices of the observed reflexions, and similar diffuse streaks are obtained. Owing to the restrictions on the indices of the observed reflexions, the relationship between the unit-cell dimensions, and the diffuse scattering on the odd-order layer lines, the zero- and odd-order layer lines of the two varieties are practically identical; but the difference is seen clearly on the even-order layer lines, owing to the different positions of the $h0l$ reflexions of the two varieties. There are also notable differences between the varieties in other respects. Whereas in clino-chrysotile $h0l$ reflexions are very weak for h odd, in ortho-chrysotile there is no restriction on h for strong reflexions with l even. Also, the proportion of

material in 'abnormal orientations' (Aruja, 1943), that is, with the fibre axis parallel to the directions [010] or [013], is either zero or very much smaller than in clino-chrysotile. It is notable that Hargreaves & Taylor (1946) found variations between Canadian and Rhodesian fibres in respect of the subsidiary layer lines, which are produced by the material in the abnormal orientations.

Further work is in progress on the structure of ortho-chrysotile and its bearing on the general problems of chrysotile structure.

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A note on the solution of the structure-factor equations. By J. KARLE and H. HAUPTMAN, *U.S. Naval Research Laboratory, Washington, D.C., U.S.A.*

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The crystal-structure problem for N point atoms per unit cell is the problem of solving for the atomic co-ordinates, x_j, y_j, z_j ($j=1, 2, \dots, N$) the system of equations

$$F_{hkl} = \sum_{j=1}^N f_j(h, k, l) \exp[-2\pi i(hx_j + ky_j + lz_j)], \quad (1)$$

where h, k, l take on various integral values. The $f_j(h, k, l)$ and only the magnitudes $|F_{hkl}|$ of the complex structure factors F_{hkl} are known from experiment. It can be shown that only the differences $x_\mu - x_\nu, y_\mu - y_\nu, z_\mu - z_\nu$ are then determined by (1), and that $3(N-1)$ independent magnitudes $|F_{hkl}|$ are sufficient to determine the solution (Hauptman & Karle, 1950).

In previous papers (Avrami, 1938; Hauptman & Karle, 1950), solutions to this problem have been obtained which require more than the algebraic minimum of data. It is the purpose of this note to show how the solution using the minimum of data may be found in principle. This solution is not developed in detail since it is very complex and appears to be unsuited for practical computation.

Each equation of (1) is multiplied by its complex conjugate, yielding

$$|F_{hkl}|^2 = \sum_{\mu, \nu}^N \sum_{\mu, \nu} f_\mu(h, k, l) f_\nu(h, k, l) \times \exp\{-2\pi i[h(x_\mu - x_\nu) + k(y_\mu - y_\nu) + l(z_\mu - z_\nu)]\}. \quad (2)$$

By making the substitution

$$\xi_\mu = \exp[-2\pi i x_\mu], \quad \eta_\mu = \exp[-2\pi i y_\mu],$$

and

$$\zeta_\mu = \exp[-2\pi i z_\mu],$$

the system (2) becomes a set of algebraic equations. This system of equations may be solved by algebraic elimination theory as follows:

Given a set of n polynomials in n unknowns,

$$g_i(w_1, w_2, \dots, w_n), \quad i=1, 2, \dots, n,$$

it is possible to replace the system of n equations, $g_i=0$, by a single algebraic equation involving one of the unknowns (van der Waerden, 1940). The roots of this algebraic equation are the possible values of this unknown. The equation is obtained in the following fashion. First we state the necessary and sufficient condition that a system of n equations in one variable, $g_i(w)=0, i=1, 2, \dots, n$,

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have a common root. Let the degree of the equation of highest degree be equal to m . Multiply each polynomial g_i of lower degree m_i by w^{m-m_i} and by $(w-1)^{m-m_i}$, thus obtaining a new system of polynomials which we adjoin to the polynomials of degree m . This results in a new system of polynomials $h_i, i=1, 2, \dots, p$, each of degree m . Clearly, if all the original polynomials are of degree m , then $p=n$; otherwise $p>n$. Next, the linear combinations

$$\left. \begin{aligned} h_u &= u_1 h_1 + \dots + u_p h_p, \\ h_v &= v_1 h_1 + \dots + v_p h_p, \end{aligned} \right\} \quad (3)$$

are constructed which, when rearranged, are seen to be polynomials in w , and the u 's and v 's are independent variables. These polynomials may be written

$$\left. \begin{aligned} h_u &= a_0 w^m + a_1 w^{m-1} + \dots + a_m, \\ h_v &= b_0 w^m + b_1 w^{m-1} + \dots + b_m, \end{aligned} \right\} \quad (4)$$

where the a 's and b 's are seen to be linear combinations of the u 's and v 's. The resultant of these two polynomials is

$$R = \begin{vmatrix} a_0 & a_1 & a_2 & \dots & a_m & 0 & 0 & \dots & 0 \\ 0 & a_0 & a_1 & \dots & a_{m-1} & a_m & 0 & \dots & 0 \\ \cdot & \cdot & \cdot & \dots & \cdot & \cdot & \cdot & \dots & \cdot \\ 0 & 0 & 0 & \dots & a_0 & a_1 & a_2 & a_3 & \dots & a_m \\ b_0 & b_1 & b_2 & \dots & b_m & 0 & 0 & \dots & 0 \\ 0 & b_0 & b_1 & \dots & b_{m-1} & b_m & 0 & \dots & 0 \\ \cdot & \cdot & \cdot & \dots & \cdot & \cdot & \cdot & \dots & \cdot \\ 0 & 0 & 0 & \dots & b_0 & b_1 & b_2 & b_3 & \dots & b_m \end{vmatrix}, \quad (5)$$

which must be identically equal to zero, i.e. the coefficient of each power $u^i v^j$ must be equal to zero. We obtain in this way a system of polynomials on the coefficients of the g_i which, when set equal to zero, are necessary and sufficient conditions that the original system of equations have a common root. This procedure, when used with the system of n equations in n unknowns

$$g_i(w_1, w_2, \dots, w_n) = 0, \quad i=1, 2, \dots, n,$$

may be applied repeatedly to eliminate successively each of the variables until we are left with one equation in one unknown, whose roots yield possible co-ordinates of one of the atoms. The main drawback of this procedure is the great complexity of carrying out the operations involved in successive eliminations.