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 orthochrysotile and its bearing on the general problems of chrysotile structure.

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A note on the solution of the structure-factor equations.

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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 $(j=1, 2, \ldots, N)$ the system of equations

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

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

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

By making the substitution

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

and

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

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,

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

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, $g_i(w)=0$, $i=1, 2, \ldots, n$, have a common root. Let the degree of the equation of highest degree be equal to m. Muitiply 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, $i=1, 2, \ldots, p$, each of degree m. Clearly, if all the original polynomials are of degree m, then $p=n$; otherwise $p>n$. Next, the linear combinations

$$\left.\begin{aligned} h_u&=u_1h_1+\ldots+u_ph_p,\\ h_v&=v_1h_1+\ldots+v_ph_p,\end{aligned}\right\} \qquad (3)$$

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

$$\left.\begin{aligned} h_u&=a_0w^m+a_1w^{m-1}+\ldots+a_m,\\ h_v&=b_0w^m+b_1w^{m-1}+\ldots+b_m,\end{aligned}\right\} \qquad (4)$$

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

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

which must be identically equal to zero, i.e. the coefficient of each power u^iv^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

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

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.

As an application of the above procedure, we consider the case of three atoms per unit cell in one dimension. Equations (2) then become

$$|F_1|^2=f_{11}^2+f_{12}^2+f_{13}^2+f_{11}f_{12}(\xi_{12}+\xi_{12}^{-1})+f_{11}f_{13}(\xi_{13}+\xi_{13}^{-1}) +f_{12}f_{13}(\xi_{12}\xi_{13}^{-1}+\xi_{12}^{-1}\xi_{13}), \quad (6)$$

$$|F_2|^2=f_{21}^2+f_{22}^2+f_{23}^2+f_{21}f_{22}(\xi_{12}^2+\xi_{12}^{-2})+f_{21}f_{23}(\xi_{13}^2+\xi_{13}^{-2}) +f_{22}f_{23}(\xi_{12}^2\xi_{13}^{-2}+\xi_{12}^{-2}\xi_{13}^2), \quad (7)$$

where $\xi_{12}=\xi_1\xi_2^{-1}=\exp[-2\pi i(x_1-x_2)]$,
and $\xi_{13}=\xi_1\xi_3^{-1}=\exp[-2\pi i(x_1-x_3)]$, (8)

so that ξ_{12} and ξ_{13} determine the x co-ordinates. If we set

$$s=\xi_{12}+\xi_{12}^{-1} \quad \text{and} \quad t=\xi_{13}+\xi_{13}^{-1}, \quad (9)$$

equations (6) and (7) may be replaced by

$$a_0t^2+a_1t+a_2=0 \quad (10)$$

and

$$b_0t^2+b_1t+b_2=0, \quad (11)$$

where

$$a_0=f_{21}f_{23}+f_{22}f_{23}f_{11}^2/f_{12}^2,$$
$$a_1=2f_{11}f_{22}f_{23}(f_{11}f_{12}s+f_{11}^2+f_{12}^2+f_{13}^2-|F_1|^2)/f_{12}^2f_{13},$$
$$a_2=f_{21}f_{22}s^2+f_{22}f_{23}(f_{11}f_{12}s+f_{11}^2+f_{12}^2+f_{13}^2-|F_1|^2)/f_{12}^2f_{13}^2 +f_{21}^2+f_{22}^2+f_{23}^2-2f_{21}f_{22}-2f_{21}f_{23}-2f_{22}f_{23}-|F_2|^2,$$
$$b_0=f_{13}f_{23}[f_{11}f_{22}s+f_{12}(f_{22}-f_{21})],$$
$$b_1=f_{22}f_{23}[f_{11}f_{12}s^2+(f_{11}^2+f_{12}^2+f_{13}^2-|F_1|^2)s],$$
$$b_2=f_{12}f_{13}[f_{22}(f_{23}-f_{21})s^2-f_{21}^2-f_{22}^2-f_{23}^2+|F_2|^2 +2f_{21}f_{22}+2f_{21}f_{23}-2f_{22}f_{23}].$$

The substitution (9) leads to simpler equations than would be obtained if the elimination theory were applied to (7) and (8) directly.

The elimination theory when applied to the quadratics (10) and (11) yields for the eliminant

$$4R=(2a_0b_2-a_1b_1+2a_2b_0)^2-(4a_0a_2-a_1^2)(4b_0b_2-b_1^2)=0. \quad (12)$$

The application of this result to equations (10) and (11) to eliminate t gives a sextic in s. Knowing s, ξ_{12} can be found from (9) and, since t is the common root of (10) and (11), ξ_{13} may also be obtained from (9).

The elimination theory is completely general and offers the solution in principle to the crystal-structure problem. However, it is seen from the foregoing treatment that the algebraic approach is very complicated and, for crystals containing several atoms in the unit cell, it appears to be impractical. The relations obtained in the previous paper (Hauptman & Karle, 1950) are eliminants of the structure-factor equations. They were obtained however by making use of the properties of hermitian forms which avoided the necessity of finding many successive eliminants.

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Utilisation de la méthode de Bragg–Brentano par l'emploi d'ampoules scellées à foyer fin.

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Dans la méthode de Bragg–Brentano appliquée à l'étude des poudres cristallines, on emploie une fente dont l''image' se forme sur le film récepteur.

On peut, comme l'a signalé Brentano (1949), explorer un domaine angulaire assez grand en imprimant une rotation à l'échantillon plan, utilisant un diaphragme qui tourne à une vitesse angulaire double de celle de l'échantillon examiné et plaçant la fente sur la circonférence de support du film. Dans ce cas, le temps d'exposition devient du même ordre de grandeur que les temps nécessaires pour obtenir un Debye–Scherrer ordinaire.

Lorsqu'on dispose d'une ampoule à foyer fin, on peut supprimer la fente et disposer l'ampoule par rapport à la caméra de telle manière que le foyer se trouve sur la circonférence de support du film. Dans ces conditions, les temps d'exposition sont fortement réduits et deviennent extrêmement intéressants.

La possibilité de disposer d'ampoules *scellées* à foyer fin supprime toutes les difficultés inhérentes aux tubes démontables et rend la méthode utilisable dans les laboratoires industriels.

Par l'emploi d'une caméra de 22,6 cm. de diamètre, nous avons pu obtenir des radiogrammes à forte dispersion en des temps relativement courts. La Fig. 1 représente les radiogrammes obtenus par réflexion sur le plan de clivage d'un monocristal de mica. La radiation Cu $K\alpha$ est partiellement filtrée de $K\beta$ au moyen d'un écran en nickel.*

Dans le cas des apatites (Fig. 2) qui nécessitent généralement des temps d'exposition assez élevés ($\sim$100 milliampères heures), les temps d'exposition nécessaires n'ont pas dépassé 10 milliampères heures. En poussant la tension de l'ampoule à 50 kV. et en utilisant des caméras de plus petit diamètre, le temps d'exposition pourrait encore être réduit notablement.

Cette méthode dont le principe n'est pas nouveau, mais qui, à notre connaissance, n'a jamais été appliquée sous cette forme, peut, à notre sens, présenter beaucoup d'intérêt pour les contrôles et les recherches. Elle n'a pas la prétention de supplanter les méthodes dans lesquelles la focalisation est parfaite mais elle présente l'avantage de pouvoir être utilisée sans appareil coûteux, encombrant, de réglage difficile et de déréglage facile. Elle peut être utilisée dans les mêmes buts que la méthode de Debye–Scherrer, pour la comparaison des intensités des divers ordres d'une réflexion et pour l'étude des molécules à longues chaînes orientées sur verre ou sur plomb.

Référence

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* L'ampoule étant en usage depuis un temps assez long, on remarque, pour chaque ordre, à côté des raies $K\alpha$ et $K\beta$ (plus faible) du cuivre, la raie L du tungstène déposé sur l'anticathode.