

reflexions is again indicative of the randomness of orientation of the layers. It appears, therefore, when meta-halloysite is formed from halloysite by low-temperature dehydration, that the H₂O layers are expelled with subsequent collapse of the randomly orientated kaolinitic layers.

The exact values of the basal spacings, (001) and (002), of meta-halloysite appear significant. Naturally occurring specimens give values for d (001) of the order of 7.3-7.5 Å., and the line is generally diffuse, mainly on the low angle side; d (002) is about 3.6 Å., so that d (001) $>$ $2 \times d$ (002). Heat treatment sharpens the (001) line considerably and reduces d (001) almost to 7.2 Å.; the (002) line also sharpens slightly but with little change of spacing. This is illustrated in the figure. It is suggested that the kaolinitic layers in meta-halloysite are originally distorted, with some layers more widely spaced than 7.2 Å., and that heat treatment causes the layers to 'settle down' into a more regular formation. This may also be correlated with MacEwan's observation that meta-halloysite formed by gentle dehydration of halloysite will combine almost completely with ethylene glycol, whereas after heat treatment this is no longer possible; this probably indicates that with heat treatment the numbers of effective linkages between the kaolinite sheets increases.

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Patterson Distributions and Native Protein Crystallography

MEGAMOLECULAR crystals such as the crystals of native proteins confront X-ray crystallography with a new situation, since the structure of the molecules is unknown. We suggest that a systematic study of what may be called the *language of structure factors* may be a useful, even a necessary, preliminary to the interpretation of the intensity maps of crystals containing megamolecules of unknown structure. A preliminary study of this nature has therefore been undertaken¹. The purpose of this note is to describe one by-product of this work which may be of interest in view of the great prominence given to the Patterson diagrams of protein crystals, namely, a method of evaluating the Patterson distribution of a given distribution.

Let $g(x)$ be a distribution in one-dimensional space satisfying appropriate conditions². Then its structure factor is

$$G(X) = \int_{-\infty}^{\infty} e^{2\pi i x X} g(x) dx$$

and

$$g(x) = \int_{-\infty}^{\infty} e^{-2\pi i x X} G(X) dX.$$

Now by definition the Patterson distribution $g_P(x)$ has the structure factor $|G(X)|^2$. Hence

$$g_P(x) = \int_{-\infty}^{\infty} e^{-2\pi i x X} |G(X)|^2 dX.$$

As an example, let $g(x)$ be 1, $\frac{1}{2}$, 0 according as x^2 is less than, equal to or greater than unity. Then

$$G(X) = \sin 2\pi X / \pi X,$$

and it follows that

$$\begin{aligned} g_P(x) &= \int_{-\infty}^{\infty} e^{-2\pi i x X} |G(X)|^2 dX \\ &= 2 \int_0^{\infty} \cos 2\pi X (\sin 2\pi X / \pi X)^2 dX. \end{aligned}$$

Using Dirichlet's discontinuous factor, we find that $g_P(x)$ is confined to the strip for which x^2 is less than 4 and within that range is given by

$$g_P(x) = 2 - |x|.$$

The method may be used also in cases in two- and three-dimensions. We may cite two examples.

Let $g(xyz)$ be a unit distribution confined to a cube volume defined by the planes $x^2 = 1$, $y^2 = 1$, $z^2 = 1$. Then, proceeding after the same manner, its structure factor is

$$\begin{aligned} G(XYZ) &= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} e^{2\pi i(xX+yY+zZ)} dx dy dz \\ &= (\sin 2\pi X \sin 2\pi Y \sin 2\pi Z) / \pi^3 XYZ. \end{aligned}$$

Now, by definition, the Patterson distribution is given by

$$g_P(xyz) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} e^{-2\pi i(xX+yY+zZ)} |G(XYZ)|^2 dX dY dZ.$$

Again making use of Dirichlet's discontinuous factor, we find that the Patterson distribution is confined to a similarly situated cube of double the dimensions and is given therein by

$$g_P(xyz) = (2 - |x|)(2 - |y|)(2 - |z|).$$

Let $g(r)$ be a spherically symmetric distribution. Then its structure factor, also spherically symmetric, is given by

$$G(R) = 4\pi \int_0^{\infty} r^2 g(r) [\sin 2\pi r R / 2\pi r R] dr,$$

as in the case of the atomic scattering factor, for example. The Patterson distribution is then

$$g_P(r) = 4\pi \int_0^{\infty} R^2 |G(R)|^2 [\sin 2\pi r R / 2\pi r R] dR.$$

If $g(r) = 1/r$ within the unit sphere and is zero outside it, then

$$G(R) = [1 - \cos 2\pi R] / \pi R^2.$$

The Patterson distribution is then

$$g_P(r) = 4\pi \int_0^{\infty} R^2 \left\{ \frac{1 - \cos 2\pi R}{\pi R^2} \right\}^2 \frac{\sin 2\pi r R}{2\pi r R} dR.$$

It follows that $g_P(r)$ is confined to a sphere of double the dimensions, being given by

$$g_P(r) = \pi(4 - 3r, r - 4 + 4/r)$$

for $r = 0$ to 1 and 1 to 2, respectively. Proceeding in the same way with

$$g(r) = a/r + b + cr + dr^2 \dots$$

we may study the anatomy of the Patterson distribution corresponding to two or more distributions superposed, analysing it into the terms due to the distributions separately and the terms due to their interactions in pairs. This analysis is of interest in connexion with all native protein crystals which are essentially protein-water systems.

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¹ "Fourier Transforms and Structure Factors." American Society for X-Ray and Electron Diffraction Monograph, No. 2 (in course of publication).

² Courant, R., "Differential and Integral Calculus," 2, 318 (Nordemann Publishing Company, New York, 1936).

Total Reflexion in Absorbing Media

It does not appear that the features of total reflexion in the case of two absorbing media have been well introduced into light, particularly a discontinuity which characterizes it, and which may provide a new method of comparing conductivities.

We consider a plane electromagnetic wave incident on a plane boundary between a medium with inductive capacity ϵ_1 , conductivity σ_1 , and a medium with ϵ_2 , σ_2 . We assume $\mu_1 = \mu_2$. Let the boundary be the $y-z$ plane; let the electric vector be perpendicular to the plane of incidence, and be represented in the two media respectively by:

$$\left. \begin{aligned} E_y^{(1)} &= E e^{-\sqrt{\epsilon_1 \mu_0} \omega [a_z x + a_z z + i b_z x + i b_z z] + i \omega t}, \\ E_y^{(2)} &= E'' e^{-\sqrt{\epsilon_2 \mu_0} \omega [A_z x + A_z z + i B_z x + i B_z z] + i \omega t} \end{aligned} \right\} (1)$$

(where $\omega = 2\pi \times$ frequency).

These quantities are connected by the relations:

$$\left. \begin{aligned} b^2 - a^2 &= 1 & ; & & B^2 - A^2 &= 1 & ; \\ 2\bar{a} \cdot \bar{b} &= \frac{\sigma_1}{\epsilon_1 \omega} = \eta_1 & ; & & 2\bar{A} \cdot \bar{B} &= \frac{\sigma_2}{\epsilon_2 \omega} = \eta_2 & ; \\ A_z &= \sqrt{\frac{\epsilon_1}{\epsilon_2}} a_z = \frac{a_z}{n} & ; & & B_z &= \sqrt{\frac{\epsilon_1}{\epsilon_2}} b_z = \frac{b_z}{n}. \end{aligned} \right\} (2)$$

by means of which, if we assume knowledge of all the parameters of the first medium, and of n and η_2 , we find: