SHORT COMMUNICATIONS

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contraction of 2% is largely in a direction normal to the shearing movement:

Parameter of $\gamma$: $a = 3.585 \, \text{Å}$;
whence $\frac{2a}{c} = 2.535 \, \text{Å}$, $\frac{3a}{c} = 4.140 \, \text{Å}$.

Parameters of $\epsilon$: $a = 2.528 \, \text{Å}$, $c = 4.080 \, \text{Å}$.

The mechanism is of the type which produces a ‘Widmanstätten’ pattern of strain bands; and the contraction associated with the transformation limits the growth of $\epsilon$ around each nucleus. A photomicrograph (Fig. 2) confirms both the strain pattern and the absence of massive precipitate, although individual phases cannot be distinguished.


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Shannon (1949), in the field of communication theory, has given the following theorem: If a function $d(x)$ is known to vanish outside the points $x = \pm a/2$, then its Fourier transform $F(X)$ is completely specified by the values which it assumes at the points $X = 0, \pm 1/a, \pm 2/a, \ldots$. In fact, the continuous $F(X)$ may be filled in merely by laying down the function $\sin \pi aX/\pi aX$ at each of the above points, with weight equal to the value of $F(X)$ at that point, and adding.

Now the electron-density function $d(x)$ describing a single unit cell of a crystal vanishes outside the points $x = \pm a/2$, where $a$ is the length of the cell. The reciprocal-lattice points are at $X = 0, \pm 1/a, \pm 2/a, \ldots$, and hence the experimentally observable values of $F(X)$ would suffice, by the theorem, to determine $F(X)$ everywhere, if the phases were known. (In principle, the necessary points extend indefinitely in reciprocal space, but by using, say, Gaussian atoms both $d(x)$ and $F(X)$ can be effectively confined to the unit cell and the observable region, respectively.)

For centrosymmetrical structures, to be able to fill in the $|F|^2$ function would require knowledge of $|F|^2$ at the half-integral $h$'s, as well as at the integral $h$'s. This is equivalent to a statement made by Gay (1951).

I think the conclusions which may be stated at this point are:

1. Direct structure determination, for centrosymmetric structures, could be accomplished as well by finding the sizes of the $|F|^2$ at half-integral $h$ as by the usual procedure of finding the signs of the $F$'s at integral $h$.

2. In work like that of Boyes-Watson, Davidson & Perutz (1947) on haemoglobin, where $|F|^2$ was observed at non-integral $h$, it would suffice to have only the values at half-integral $h$.

The extension to three dimensions is obvious.

References


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The data presented here form part of an extended survey of crystalline peptides recently begun by the Wool Industries Research Association. The objects of the investigation are first to obtain some knowledge of the factors influencing the crystallization of these materials; secondly, from their unit-cell dimensions to obtain information regarding the types of molecular arrangements present, and thirdly to select materials suitable for a more detailed X-ray examination.

Source of peptides.

Glycyl-L-tyrosine was obtained from Roche Products, Welwyn Garden City, England, and the monohydrochloride was prepared from it by treatment with excess of 2N.HCl, followed by evaporation at room temperature.

(Found 12.1% Cl; calculated 12.9%.)

Glycyl-DL-leucine and glycyl-DL-serine were synthesized by the chloracetyl chloride method first described by