

slight shortening of the second disorientation spacing, then a change towards (3) would take place. The probability of occurrence of two adjacent disorientations is equal to $p^2(1-p)$ and it is, in fact, found that improved agreement over an increased range of p can be obtained by adding a further term, $0.03p^2(1-p)$, to the right-hand side of (2).

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Short Communications

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Acta Cryst. (1951). **4**, 561

The a dimension of graphite. By G. E. BACON, *Atomic Energy Research Establishment, Harwell, Didcot, England*, and R. E. FRANKLIN, *Wheatstone Physics Laboratory, King's College, London W.C. 2, England*

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It was previously reported (Bacon, 1950) that accurate measurements of the position of the $(12\bar{3}0)$ line for different graphites indicated an apparent slight variation of the a dimension. At the same time, however, measurements of the $(12\bar{3}1)$ line gave a constant a value, suggesting that, in accordance with theoretical work (Bradburn, Coulson & Rushbrooke, 1948), the true a dimension, for this range of graphites, is constant.

The anomalously low values of a obtained from the $(hki0)$ lines can be explained in exactly the same way as the displacement shown by Warren (1941) to occur in the maxima of the (hk) bands in random-layer structures. All the graphites examined in the work referred to above were imperfectly crystalline, the degree of disorder between neighbouring layers being such that the intensity of $(hki0)$ reflexions in reciprocal space always falls off much less rapidly along the c^* axis than perpendicular to it. This is illustrated in Fig. 1, which shows schematically the reciprocal space in the neighbourhood of an $(hki0)$ point.

The case of the least-crystalline sample, A_1 , of those previously measured may be considered semi-quantitatively. The breadth of the $(11\bar{2}0)$ line leads to an estimated layer diameter, b , of 1500 Å. (although the line broadening is too small for this to be determined accurately). The shape of the $(11\bar{2}4)$ line for this sample is in agreement with the hypothesis (Franklin, 1951) of a random distribution of oriented and disoriented layers, and indicates a fraction 0.2 of disorientations (Bacon, 1951). Using these figures it is found that the intensities of the streak at Q_0 and Q (Fig. 1) have fallen only to 90 and 83% of the intensity at the equator. Consequently, the displacement of the maximum of the $(11\bar{2}0)$ line will be almost as large as for a random-layer structure having layers of the same diameter.

Warren (1941) shows that the displacement in the latter case is such that the difference between the true and apparent spacings is given by

$$\Delta d = d \frac{0.16\lambda}{b \sin \theta},$$

where d is the true spacing. Applying this equation to the $(11\bar{2}0)$ line of the sample A_1 , we find that the

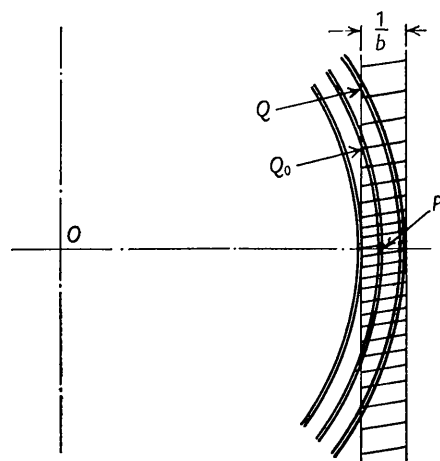


Fig. 1. $OP_0 = \frac{1}{d} = \frac{2 \sin \theta}{\lambda}$.

difference between the true and apparent values of the lattice parameter, a , is 0.0007 Å. This is exactly equal to the experimental difference between the apparent a values given by the $(11\bar{2}0)$ lines of A_1 and of a much more highly crystalline graphite, A_3 (Bacon, 1950).

The precise agreement is, of course, fortuitous, but it

is of interest to note that anomalously small values of a can be accounted for in this way, even when three-dimensional order is, as in this case, relatively highly developed.

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The determination of interplanar spacings and cell dimensions from powder photographs using an internal standard. By K. W. ANDREWS, *United Steel Companies Ltd., Research and Development Department, Stocksbridge, near Sheffield, England*

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A method for the determination of the unit-cell dimensions of non-cubic substances has been described by Bacon (1948). The object of this communication is to draw attention to some more general applications of the same simple principles which have been in use in this laboratory.

I. The simplest way of obtaining corrected interplanar spacings of a non-cubic substance is to mix it with a suitable cubic standard. Whatever method of extrapolation is employed for the cubic lattice spacings, the extrapolation curve can be used directly to give the correction to be placed on the values obtained for the interplanar spacings of the intervening non-cubic lines. From these spacings the unit-cell dimensions may be calculated as suggested by Bacon (1948).

II. An extension of this simple procedure was suggested by Jay (1942) who showed that, provided the reflected rays come from the outer layers of the specimen (thus necessitating the use of a thicker and denser specimen for materials of lower absorption), a very nearly linear extrapolation could be obtained by plotting cubic lattice spacings against $\cos^2 \theta / \sin \theta$. This function gives extrapolations which are, in effect, practically indistinguishable from those obtained with the function

$$\frac{1}{2} \left(\frac{\cos^2 \theta}{\sin \theta} + \frac{\cos^2 \theta}{\theta} \right)$$

as suggested by Nelson & Riley (1945) and by Taylor & Sinclair (1945). These functions, on extrapolation, tend to infinity as $\theta \rightarrow 0$, and direct use for correcting low-angle spacings, especially at values of θ lower than that for the cubic line of lowest spacing on the film, is limited. If, however, $(\Delta a/a) \times 100 \times \sin \theta$, where $\Delta a = a_0 - a$, is plotted against $\cos^2 \theta$, as indicated in Fig. 1, a curve, *A*, is obtained which reaches a finite value at $\cos^2 \theta = 1$. From this curve a 'percentage correction' curve, *B*, is deduced by dividing the ordinate for selected points on *A* by the value of $\sin \theta$ for these points, which are themselves conveniently chosen so that $\sin \theta = 0.1, 0.2, 0.3$, etc. (i.e. $\cos^2 \theta = 0.99, 0.96, 0.91$, etc.). The curve *A* also provides a check on the accuracy of the preliminary cubic extrapolation, and is often very nearly linear.

III. Occasionally the 'internal standard' is one of the components of a mixture, and is not cubic. In this case the interplanar spacings of the standard substance can be used to obtain a curve of $(\Delta d/d) \sin \theta$ plotted against $\cos^2 \theta$.

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IV. If the curve of $(\Delta d/d) \sin \theta$ is obtained for some non-cubic substances and it does not pass through the origin but intersects the vertical axis above or below zero, at $\cos^2 \theta = 0$, this result may be useful for estimating solid-solution effects in compounds where the interplanar spacings for the pure compound are known to a sufficient degree of accuracy. Thus $\Delta d/d = \Delta d_1/d + \Delta d_2/d$ and the intercept represented by $\Delta d_1/d$ is the magnitude of the solid-solution effect, whilst $(\Delta d_2/d) \sin \theta$ would give an

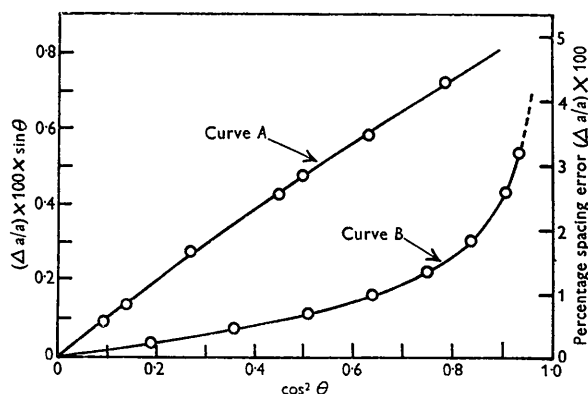


Fig. 1. Curve *A*: the relationship of $(\Delta a/a) \times 100 \times \sin \theta$ to $\cos^2 \theta$ for a specimen containing MgO. Curve *B*: the curve of percentage spacing error against $\cos^2 \theta$ derived from curve *A*. The individual points correspond to $\sin \theta = 0.2, 0.3, 0.4$, etc. (i.e. $\cos^2 \theta = 0.96, 0.91, 0.84, 0.75$, etc.).

almost linear curve through the origin if plotted against $\cos^2 \theta$. Small amounts of solid solution have been estimated in rhombohedral oxides and calcites by this method, although it is not suitable if there are marked axial-ratio changes.

V. In cases where only low- to medium-angle reflexions are suitable for measurements a correction can be applied by another simple procedure. The line separation is multiplied by the interplanar spacing for each of the standard lines and the product is plotted against the separation distance itself, as in Fig. 2. Interplanar spacings corresponding to the intervening lines are found by reading the value of the product, distance \times spacing, and dividing the product by the distance.

VI. A similar method frequently used for flat films, but of general application, is to draw a graph of the re-