If the P_n and R_n matrices are not singular they can be inverted and can be written

$$P_n^{-1}\mathbf{a}_n = A_n^s\mathbf{e}_e \qquad (7)$$

$$R_n^{-1}\mathbf{b}_n = A_n^s\mathbf{e}_0 \,. \qquad (8)$$

Because the first element of vector $\mathbf{e}_e$ is the zero-order moment of e_L (the matrix P_n has so been chosen) the first element of vector $P_n^{-1}\mathbf{a}_n$ defines the particle-size coefficients A_n^s. So by computing the inverse of matrix P_n it is possible to determine the particle-size coefficients A_n^s and the deformation moments $\langle e_L^k\rangle$ at the same time.

During the separation of particle-size and deformation coefficients it was supposed that the average crystal shape is spherical, *e.g.* that A_n^s is independent of h_0. If the particle shape cannot be supposed to be isotropic in this sense or if in case of anisotropy the explicit form of function $A_n^s(h_0)$ is unknown, the separation of particle-size and deformation coefficients has no physical meaning.

Obviously if in equation (1) only second-order terms are considered, the method described for separating particle size and deformation coefficients is identical with Warren's (1959) method.

The author wishes to thank Dr L. Zsoldos for comments on the manuscript.

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The determination of strain distributions and particle-size coefficient by the moment method.

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The moment method has previously been shown to yield the strain distribution in a crystal from measurements of broadened diffraction lines under the assumption that all broadening was due to strain. Ungár has pointed out that such an assumption is unnecessary, but his method involves sacrificing the determination of the highest strain moment consistent with the number of experimentally measured diffraction orders. It is shown in the present paper that such a sacrifice can lead to serious error in certain cases. A simple scheme is described which extracts the maximum amount of information from the observed data to give both the strain distribution and the particle-size coefficient.

In a previous paper (Harrison, 1966) it was shown that the strain distribution in a deformed crystal can be determined from measurements of broadened diffraction lines under the assumption that no particle-size effects contribute to the broadening. Ungár (1967) has since pointed out that such an assumption is unnecessary, but his method, which leads to a determination of the 'particle-size' coefficient, does so at the expense of determining one of the high-order deformation moments.

Summary of the previous methods

Harrison employed the truncated expansions

$$a_i' = 1 + \sum_{j=1}^{m} P_{i,j}\langle e^{2j}\rangle \qquad i=1,2,\ldots m$$

$$b_i' = \sum_{j=1}^{m} R_{i,j}\langle e^{2j-1}\rangle$$

m = number of observed diffraction orders

to determine the deformation moments $\langle e^k\rangle$ of the strain distribution from the cosine and sine coefficients a_i' and b_i' of the Fourier expansion of the broadened diffraction line (the dashes denoting that the coefficients are from a line broadened by strain alone). The matrix elements $P_{i,j}$ and $R_{i,j}$ are given by

$$P_{i,j} = \frac{(-1)^j}{(2j)!}\,(2\pi L h_{i,0/a})^{2j}$$

$$R_{i,j} = \frac{(-1)^j}{(2j-1)!}\,(2\pi L h_{i,0/a})^{2j-1}$$

where $h_{i,0}^2 = h_i^2 + k_i^2 + l_i^2$
and the deformation moments are then computed by a process of matrix inversion to give

$$\langle e^{2j}\rangle = \sum_{i=1}^{m} P_{i,j}^{-1}(a_i' - 1) \qquad j=1,2,\ldots m$$

$$\langle e^{2j-1}\rangle = \sum_{i=1}^{m} R_{i,j}^{-1} b_i'$$

so that the first $2m$ moments may be obtained from measurements of m diffracted orders.

Ungár waives assumptions about the sources of strain broadening and writes

$$a_i = A_n^s + A_n^s \sum_{j=1}^{m-1} P_{i,j}\langle e^{2j}\rangle \qquad i=1,2,\ldots m$$

$$b_i = A_n^s \sum_{j=1}^{m} R_{i,j}\langle e^{2j-1}\rangle$$

m = the number of observed diffraction orders

where the a_i and b_i are the measured Fourier coefficients and A_n^s is the particle size coefficient. The cosine expansion is now truncated at the $(2m-2)$th moment to enable A_n^s to be calculated with the first $m-1$ even moments from the m equations for a_i. The first m odd moments may then be calculated from the equations for the b_i. This method will be quite satisfactory provided the $2m$th moment can be ignored. Unfortunately, as a numerical example will show, this is not always so.

Numerical example

Examples of artificial strain distributions were described in a previous paper (Harrison, 1966) and cases 1 and 4 of that paper will be taken as illustrations of the following discussion. For simplicity we shall consider the effect of ignoring the highest even-order moment in computing the strain distribution at the origin, that is $S(0)$, where $S(e)$ is the function giving the distribution of strain e. For case 1 (see Fig. 2 of previous paper) the value of $S(0)$ computed from six deformation moments up to $\langle e^6 \rangle$ was 118·6. The same computation performed using only moments up to $\langle e^5 \rangle$ gave $S(0)=116{\cdot}3$ (the real value of $S(0)=118$). The error here, at least at the origin of $S(e)$ is negligible. However, for case 4 (where the real value of $S(0)=230$) similar computations gave $S(0)=189{\cdot}4$ for the six moment case and $S(0)=153{\cdot}8$ in the case of five moments. The error now is serious.

The use of a combination of both methods

Since neither of the above methods seems to extract the maximum amount of information from the experimental data the following scheme is proposed which preserves the advantages of both without impairing the accuracy of either. We first define the set of m ratios g_i where

$$g_i = a_i/a_j \qquad \begin{array}{l} i=1,2,\ldots m \\ j=i+1,\, i\neq m \\ j=1,\, i=m \\ m=\text{number of measured orders} \end{array}$$

the a_i being the measured cosine coefficients of the broadened line. The g_i are thus independent of the 'particle-size' coefficients A_n^s, if, as has been assumed hitherto, the a_i are represented by the simple product $A_n^D A_n^s$ where A_n^D is the distortion component of the cosine coefficient.

Then

$$g_i = \frac{1+\sum\limits_{k=1}^{m} P_{i,k}\langle e^{2k}\rangle}{1+\sum\limits_{k=1}^{m} P_{j,k}\langle e^{2k}\rangle} \qquad \begin{array}{l} j=i+1,\, i\neq m \\ j=1,\, i=m \end{array}$$

where the $P_{i,k}$ are the same as those defined above and

$$g_i - 1 = \sum_{k=1}^{m} (P_{i,k} - g_i P_{j,k})\langle e^{2k}\rangle\,,$$

whence we find

$$\langle e^{2k}\rangle = \sum_i (P_{i,k} - g_i P_{j,k})^{-1}(g_i - 1)$$

where $(P_{i,k} - g_i P_{j,k})^{-1}$ are the elements of the inverse matrix. Thus are determined the first m even deformation moments. The 'particle-size' coefficient may now be determined from

$$A_n^s = \frac{a_1}{1+\sum\limits_{j=1}^{m} P_{i,j}\langle e^{2j}\rangle}\,.$$

The odd deformation moments then follow from the equations

$$b_i = A_n^s \sum_{j=1}^{m} R_{i,j}\langle e^{2j-1}\rangle \qquad i=1,2,\ldots m$$

Conclusion

When the ratios of the Fourier cosine coefficients are used in the moment method to determine the even order moments it is possible to obtain the 'particle size' coefficient as well as the strain distribution function.

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Crystallography of two modifications of 10-hydroxy-10,9-borazarophenanthrene.

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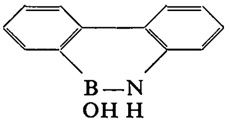
Two polymorphic modifications of 10-hydroxy-10,9-borazarophenanthrene were obtained; the transformation of form I into form II, and *vice versa*, could be observed. The crystals of form I are monoclinic, in the space group Cc or $C2/c$. The unit-cell constants are: $a=49{\cdot}6\pm0{\cdot}1$, $b=5{\cdot}5\pm0{\cdot}1$, $c=13{\cdot}2\pm0{\cdot}1$ Å; $\beta=93°$; $Z=16$. Density: 1·44 g.cm^{-3}. The crystals of form II are monoclinic in the space group $P2_1/a$ The unit-cell constants are: $a=28{\cdot}4\pm0{\cdot}1$, $b=5{\cdot}2\pm0{\cdot}1$, $c=12{\cdot}7\pm0{\cdot}1$ Å; $\beta=92°30'$; $Z=8$ Density$=1{\cdot}38$ g.cm^{-3}

The purpose of this note is to present the results obtained in the crystal study of two polymorphic modifications of 10-hydroxy-10,9-borazarophenanthrene, $C_{12}H_{10}OBN$,



one of the heterocyclic compounds synthesized at the Department of Molecular and Atomic Physics, Argentine Atomic Energy Commission*. The sample was prepared according to Dewar, Kubba & Pettit (1958) by boiling under reflux a benzene solution of 2-aminobiphenyl and boron

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* Sample prepared by Dr Marcelo Molinari.