will be quite satisfactory provided the 2mth 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

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

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

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

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

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

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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References

Harrison, J. W. (1966). *Acta Cryst.* **20**, 390.
Ungár, T. H. (1967). *Acta Cryst.* **23**, 174.

Acta Cryst. (1967). **23**, 176

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

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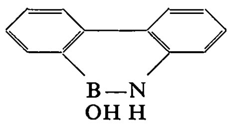
Two polymorphic modifications of 10-hydroxy-10,9-borazarophenanthrene were obtained; the transformation of form I into form II, and *vice versa*, could be observed. The crystals of form I are monoclinic, in the space group Cc or $C2/c$. The unit-cell constants are: $a=49{\cdot}6\pm0{\cdot}1$, $b=5{\cdot}5\pm0{\cdot}1$, $c=13{\cdot}2\pm0{\cdot}1$ 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.

trichloride, and subsequent hydrolysis at room temperature. This sample was labelled form I.

By slow evaporation at room temperature of a solution of form I in an ethanol–water mixture, different crystals were obtained; these were labelled form II.

Rotation, Weissenberg and precession photographs were obtained with Ni-filtered Cu *K* radiation.

The crystal data are as follows:

Form I:
System monoclinic
Space group either *Cc* or *C*2/*c* from the following systematic absences:

hkl for $h+k=2n+1$
$h0l$ for $l=2n+1$.
$a=49\cdot6\pm0\cdot1$ Å
$b=\ 5\cdot5\pm0\cdot1$
$c=13\cdot2\pm0\cdot1$
$\beta=93°$
$Z=16$
$D_x=1\cdot44$ g.cm^{-3}
D_m (pycnometer) $=1\cdot43\pm0\cdot01$ g.cm^{-3} .

The crystals grew in the form of very small needles.

Form II
System: monoclinic
Space group $P2_1/a$ from the following systematic absences:

$h0l$ for $h=2n+1$
$0k0$ for $k=2n+1$
$a=28\cdot4\pm0\cdot1$ Å
$b=\ 5\cdot2\pm0\cdot1$
$c=12\cdot7\pm0\cdot1$
$\beta=92°30'$
$Z=8$
$D_x=1\cdot38$ g.cm^{-3}
D_m (flotation) $=1\cdot35\pm0\cdot01$ g.cm^{-3} .

The crystals grew in the form of needles.

The powder data for both forms are being submitted for inclusion in the ASTM X-ray Powder Data File.

Micro-melting points were determined on a Kofler hot stage to characterize both kind of crystals. Two different behaviours were observed: crystals of form I melt without decomposition at 168°C; some sublimation is observed. On the other hand when crystals of form II are gradually heated a strong sublimation is observed and, at about 80°C, the crystals alter, cracking and becoming opaque; the altered crystals melt at 168°C.

If crystals of form II are placed on a hot stage preheated to about 100°C, their melting at 125°C can be observed; on continued heating, small crystals appear in the molten mass which grow slowly and melt at 168°C.

Through the introduction of a solution phase it was possible to observe the passage of form I to form II and *vice versa*. When a saturated solution of the substance in nitrobenzene kept at 65°C was seeded with one crystal of each form, the crystals of form I grew while the crystals of form II dissolved. When the test was repeated at 32°C the process was reversed, the form II crystals growing, while the form I crystals disappeared.

References

Dewar, M. J. S., Kubba, V. P. & Pettit, R. (1958). *J. Chem. Soc.* p. 3075.

Acta Cryst. (1967). **23**, 177

Note on the structures of $TbFe_2$ and $TbFe_3$.

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By means of single-crystal X-ray diffraction methods the existence of $TbFe_3$ ($R\bar{3}m$, $PuNi_3$-type) $a=8\cdot48$ Å, $\alpha=34°20'$ has been established and that of the previously reported $TbFe_2$ ($Fd3m$, $MgCu_2$-type) $a=7\cdot40$ Å has been confirmed. Similar investigation of alloys of composition intermediate between the two compounds shows $TbFe_3$ to exist over a range of composition.

Recently Smith & Hansen (1965), by single-crystal techniques, found that the crystal structures of YNi_3, YCo_3, $ThFe_3$ and $GdFe_3$ are all isotypic with $PuNi_3$ ($R\bar{3}m$) (Cromer & Olsen, 1959). Furthermore, these authors were able to show that the erroneous interpretation of the structures by the previous investigators (Florio, Baenziger & Rundle, 1956) was due to the fault-stacking and twinning inherent to these compounds. Concurrently, based on powder pattern methods, GdX_3 and YX_3 (X = Fe, Co, Ni) (Van Vucht, 1965) and RCo_3 (R = Y, Ce, Pr, Nd, Gd, Tb, Dy, Ho, Er and Tm) (Bertaut, Lemaire & Schweizer, 1965) have all been identified as isotypic with $PuNi_3$ ($R\bar{3}m$). Also, it has been shown by means of powder pattern methods (Dwight, 1961; Novy, Vickery & Kleber, 1961; Kripyakevich, Teslyuk & Frankevich, 1965) that all the AB_2 compounds found in the R–X (R = rare earth, X = Fe, Co and Ni) systems are of the *C*15 ($MgCu_2$) type. These facts suggest that RX_2 ($Fd3m$) and RX_3 ($R\bar{3}m$) compounds coexist in the R–X systems.

A close comparison of the crystal structures of RX_2 and RX_3 compounds shows (1) the tetrahedral clustering of the X atoms as well as the stacking of these tetrahedral units in the two structures are closely related (Fig. 1) and (2) the hexagonal arrangements of the R atoms in the two structures have a common stacking sequence, *ABCABC*; the only difference is that the hexagonal array of R atoms is double layered in RX_2 and triple layered in RX_3. Inasmuch as the c/a (hexagonal representation) ratio of RX_3 compounds (4·84) is about twice that of RX_2 coumponds (2·45) and the atomic arrangements are closely related, the powder patterns of the two types of compounds are necessarily similar. This implies that it is possible to misidentify RX_3 as RX_2 based on powder pattern methods. Parallel to these

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