

contribute appreciably to the value of the pseudo-temperature factor and none should be ignored.

In the above treatment we have avoided making an explicit assumption concerning the form of ϵ_{ij}^A . It would be quite easy to substitute the specific form assumed by Borie and others, writing $\epsilon_{ij}^A = c_i r_{ij} / |r_{ij}|^3$. Then, following Borie, the summations over \mathbf{k} and \mathbf{l} not involving order parameters may be explicitly evaluated.

The task of sorting out in practice the relative importance of the various terms and the values of the correlation and displacement parameters involved in the expressions for the pseudo-temperature factor of Bragg peaks and the diffuse scattering is a difficult one. However considerable progress may be possible in particular cases if a series of measurements is made for different values of the adjustable parameters. The temperature may be varied. Variation of the composition may include use of the 50:50 composition, for which all odd-order correlation parameters vanish. Finally the scattering factors may be varied independently of all other parameters by choosing different radiations. For copper-gold alloys, for example, the condition $F_A = F_B$ is very nearly achieved in neutron diffraction and could be made exact by use of isotopically enriched elements. For this case it is interesting to note the prediction of equation (27) that a weak, broadened, short-range order peak should still appear. Measurement of such a peak would give values for the displacement parameters if the s.r.o. parameters were known, and *vice versa*.

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References

- BORIE, B. (1957). *Acta Cryst.* **10**, 89.
 BORIE, B. (1959). *Acta Cryst.* **12**, 280.
 CLAPP, P. C. (1967). In the press.
 CLAPP, P. C. & MOSS, S. C. (1966). *Phys. Rev.* **142**, 418.
 CLAPP, P. C. & MOSS, S. C. (1968). In the press.
 COCHRAN, W. & KARTHA, G. (1956). *Acta Cryst.* **9**, 941.
 COWLEY, J. M. (1950). *J. Appl. Phys.* **21**, 24.
 COWLEY, J. M. (1965). *Phys. Rev.* **138**, A1384.
 COWLEY, J. M. (1966). *J. Aust. Inst. Metals*, **11**, 258.
 COWLEY, J. M. & MURRAY, R. J. (1968). *Acta Cryst.* **A24**, 329.
 FISHER, P. M. J. (1965). *Electron Diffraction and Crystal Defects*, Melbourne.
 FLINN, P. A. (1956). *Phys. Rev.* **104**, 350.
 GEHLEN, P. & COHEN, J. B. (1965). *Phys. Rev.* **139**, A844.
 GUINIER, A. (1963). *X-ray Diffraction in Crystals, Imperfect Crystals and Amorphous Bodies*. San Francisco: Freeman and Company.
 HUANG, K. (1947). *Proc. Roy. Soc. A* **190**, 102.
 KRIVOGLAZ, M. A. (1958). *Soviet Phys. - J.E.T.P.* **1**, 1395.
 KRIVOGLAZ, M. A. & TIKHONOVA, E. A. (1960). *Ukr. Fiz. Zh.* **5**, 158.
 MOSS, S. C. (1964). *J. Appl. Phys.* **35**, 3547.
 ROBERTS, B. W. (1954). *Acta Metallurg.* **2**, 597.
 SMIRNOV, A. A. & TIKHONOVA, E. A. (1960). *Soviet Physics - Solid State* **3**, 899.
 WALKER, C. B. & KEATING, D. T. (1961). *Acta Cryst.* **14**, 1170.
 WARREN, B. E., AVERBACH, B. L. & ROBERTS, B. W. (1951). *J. Appl. Phys.* **22**, 1493.

Acta Cryst. (1968). **A24**, 563

Elastic Coefficients in Crystals

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Jahn's method of reduction of a representation has been applied and extended to obtain the fourth order and the fifth order elastic coefficients for the 32 classes of crystals.

It is well known that the character method (Bhagavan-tam & Suryanarayana, 1949) could be successfully employed for deriving the number of independent constants in respect of the various physical properties for the 32 crystal classes. Following the suggestion of Chelam (1961), one of us (Krishnamurty, 1963) has applied the character method for obtaining the number

of independent fourth-order elastic coefficients for the 32 crystallographic point groups.

In this note, it is proposed to apply and extend Jahn's (1949) method of reduction of a representation to derive the number of the fourth-order and the fifth-order elastic coefficients, which are symmetric in all the indices, for the 32 point groups. The results so ob-

Table 1. *Reduced forms of representation of polar vectors*

No.	Representation	Reduced form of the representation	Number of constants of an isotropic solid, R_∞^t
1.	$[[V^2]_4]$	$4D_0^g + 5D_2^g + D_3^g + 4D_4^g + D_5^g + 2D_6^g + D_8^g$	4
2.	$[[V^2]_5]$	$5D_0^g + 7D_2^g + 2D_3^g + 6D_4^g + 2D_5^g + 4D_6^g + D_7^g + 2D_8^g + D_{10}^g$	5

tained in respect of the fourth-order elasticity are in complete agreement with those obtained earlier by one of us (Krishnamurty, 1963). The number of the fifth-order elastic coefficients for each one of the 32 classes of crystals is worked out here for the first time.

If V denotes the representation of a polar vector, and Tisza's (1933) notation, for the symmetrical product $[V^2]$ of V with itself, is employed, one can extend the method of Jahn (1949) to higher symmetrical powers of a reducible representation. In the fourth and fifth symmetrical powers of a reducible representation, one needs the values of $[D_2^4]$ and $[D_2^5]$. They may be derived easily and are given by

$$[D_2^4] = D_0 + 2D_2 + 2D_4 + D_5 + D_6 + D_8,$$

and

$$[D_2^5] = D_0 + 2D_2 + D_3 + 2D_4 + D_5 + 2D_6 + D_7 + D_8 + D_{10}.$$

The reduced forms of the representation for the symmetrical fourth and fifth powers of $[V^2]$ are given in Table 1.

The number of constants for an isotropic solid (R_∞^t) describing the elastic coefficients is given by the coefficient of D_0^g in the reduced form of the appropriate representation in Table 1.

Since each one of the 32 crystallographic point groups is a sub-group of R_∞^t (group of all rotations and reflexions), the appropriate number of independent constants for a crystallographic point group can be obtained if the reduced form of D_L^g (which is of dimension $2L+1$ and which is even with respect to inversion) is known for the point group under consideration. The following (Jahn, 1949) is the reduction of D_L^g for the axial groups:

$C_\infty V$:

$$D_L^g = \left\{ \begin{matrix} A_1 \\ A_2 \end{matrix} \right\} + E_1 + E_2 + \dots + E_L \text{ for } L \begin{cases} \text{even} \\ \text{odd} \end{cases},$$

D_∞^h :

$$D_L^g = \left\{ \begin{matrix} A'_1 \\ A'_2 \end{matrix} \right\} + E'_1 + E'_2 + E'_3 + \dots + \left\{ \begin{matrix} E'_L \\ E'_L \end{matrix} \right\} \text{ for } L \begin{cases} \text{even} \\ \text{odd} \end{cases},$$

D_∞ :

$$D_L^g = \left\{ \begin{matrix} A_1 \\ A_2 \end{matrix} \right\} + E_1 + E_2 + \dots + E_L \text{ for } L \begin{cases} \text{even} \\ \text{odd} \end{cases}.$$

The reduced form of D_L^g for the point group ($\bar{4}3m$) has been already given by Jahn (1938), and that of the point group ($\bar{4}2m$) is given below:

$$\begin{aligned} D_0^g &= A_1, \\ D_1^g &= A_2 + E_1, \\ D_2^g &= A_1 + B_1 + B_2 + E_1, \\ D_3^g &= A_2 + B_1 + B_2 + 2E_1, \\ D_4^g &= 2A_1 + A_2 + B_1 + B_2 + 2E_1, \\ D_5^g &= A_1 + 2A_2 + B_1 + B_2 + 3E_1, \\ D_6^g &= 2A_1 + A_2 + 2B_1 + 2B_2 + 3E_1, \\ D_7^g &= A_1 + 2A_2 + 2B_1 + 2B_2 + 4E_1, \\ D_8^g &= 3A_1 + 2A_2 + 2B_1 + 2B_2 + 4E_1, \\ D_9^g &= 2A_1 + 3A_2 + 2B_1 + 2B_2 + 5E_1, \\ D_{10}^g &= 3A_1 + 2A_2 + 3B_1 + 3B_2 + 5E_1. \end{aligned}$$

Using the above reductions of D_L^g for the axial groups, and the point groups $\bar{4}3m$ and $\bar{4}2m$, the number of independent fourth order and fifth order elastic coefficients, which are given below, can be obtained for the 32 point groups:

1, $\bar{1}$: 126 (252); m , 2, $2/m$: 70 (136); $2mm$, 222 , $2/m\ 2/m\ 2/m$: 42 (78); 4, $4/m$, $\bar{4}$: 36 (68); $4mm$, $\bar{4}2m$, 422 , $4/m\ 2/m\ 2/m$: 25 (44); 3, $\bar{3}$: 42 (84); $3m$, 32 , $\bar{3}2/m$: 28 (52); $3/m$, 6, $6/m$: 24 (46); $\bar{6}2m$, $6mm$, 622 , $6/m\ 2/m\ 2/m$: 19 (33); 23, $2/m\ \bar{3}$: 14 (26); $\bar{4}3m$, 432, $4/m\ \bar{3}\ 2/m$: 11 (18).

Here the numbers inside the brackets are the appropriate number of constants for the fifth order elasticity.

It is interesting to note that in respect of higher order elasticity, the 32 crystal classes divide themselves into 11 groups. We once again observe that the five cubic classes have split themselves into 2 groups requiring different numbers of constants. This is due to the presence of additional symmetry operations S_4 or C_4 present in the point group $\bar{4}3m$ or 432 respectively. These additional symmetry operations give a smaller number of elastic coefficients involving higher order tensors for the point groups $\bar{4}3m$, 432 and $4/m\ \bar{3}\ 2/m$.

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References

- BHAGAVANTAM, S. & SURYANARAYANA, D. (1949). *Acta Cryst.* **2**, 21.
 CHELAM, E. V. (1961). Thesis submitted to the Indian Institute of Science, Bangalore.
 JAHN, H. A. (1938). *Proc. Roy. Soc. A* **168**, 469.
 JAHN, H. A. (1949). *Acta Cryst.* **2**, 30.
 KRISHNAMURTY, T. S. G. (1963). *Acta Cryst.* **16**, 839.
 TISZA, L. (1933). *Z. Phys.* **82**, 48.