QUICK ENUMERATION OF INDEPENDENT TENSOR COMPONENTS OF PHYSICAL PROPERTIES OF CRYSTALS IN TRIGONAL AND HEXAGONAL POINT GROUPS*

B. K. RAY *and* G. D. NIGAM

Department of Physics, Indian Institute of Technology, Kharagpur – 721 302

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A method determining, in a simple way, the number of non-zero independent tensor (any rank) components of a physical property of crystals is presented here. To simplify the representation of the symmetry elements, the method utilizes a transformation of coordinates in which the transformation matrix is the inverse of the eigenvector matrix of the rotational symmetry. The method is illustrated with fourth rank elastic tensor in the presence of point groups of trigonal and hexagonal systems. Like the conventional analytical method, the present method also locates the non-zero components of the tensor.

INTRODUCTION

IT is well known (Nye, 1969) that the symmetry of the crystal reduces the number of independent tensor components of a physical property. The usual procedure is to expand the invariance relation directly, but the calculations are tedious when the rank of the tensor is high. The direct inspection method (Fumi, 1952) is quick and easy but not applicable to the trigonal and hexagonal systems due evidently for the increase in the number of elements in the representation of the rotational symmetry in the conventional way. Group theoretical methods as developed by Jahn (1949), and Bhagvantam & Venkatarayudu (1951) determine only the total number of independent components. Only Landau & Lifchitz (1959) and Dieulesaint & Royer (1972) used change of coordinates.

The present method uses a transformation of axes, which diagonalises the representation of the rotational symmetry and does not complicate the representation of other symmetries. Non-zero components are those which are unaffected by the symmetry transformation in new coordinate system.

THEORY

Let us consider an n-fold axis of rotation ($n > 0$) parallel to ox_3 of an orthogonal coordinate system $ox_1x_2x_3$. The rotation matrix is

$$\mathbf{A}(n) = \left\langle \begin{matrix} \cos\theta & \sin\theta & 0 \\ -\sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{matrix} \right\rangle, \quad \ldots \quad (1)$$

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where $\theta = 2\pi/n$. For a crystal with an n-fold axis of symmetry, the invariance condition for elastic stiffness constants (which is a fourth rank tensor) is given by

$$C_{ijkl} = A_{ip}(n)\ A_{jq}(n)\ A_{kr}(n)\ A_{ls}\ C_{pqrs} \quad \ldots \quad (2)$$

Eqn. (2) is difficult to handle because the matrix $\mathbf{A}(n)$, in general, is not simple.

In the present method, the authors express the invariance relation (2) in a new coordinate system $0\ \xi_1\xi_3\xi_3$, defined by

$$\xi = \alpha \mathbf{x}, \quad \ldots \quad (3)$$

where

$$\alpha = \begin{pmatrix} 1/\sqrt{2} & i/\sqrt{2} & 0 \\ 1/\sqrt{2} & -i/\sqrt{2} & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad \ldots \quad (4)$$

which is the inverse of the eigenvector matrix of the rotation matrix $\mathbf{A}(n)$. The rotation matrix $\mathbf{A}'(n)$ in the new coordinate system is given by

$$\mathbf{A}'(n) = \alpha \mathbf{A}(n)\, \alpha^{-1} = \begin{pmatrix} \exp(i\theta) & 0 & 0 \\ 0 & \exp(i\theta) & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad \ldots \quad (5)$$

and is diagonal (cf. Goldstein, 1959). The invariance relation for the new elastic constants Γ_{ijkl} in the new coordinate system $0\ \xi_1\xi_2\xi_3$ is

$$\Gamma_{ijkl} = A'_{ii}(n)\ A'_{jj}(n)\ A'_{kk}(n)\ A'_{ll}(n)\ \Gamma_{ijkl}. \quad \ldots \quad (6)$$

The only Γ_{ijkl} different from zero are those in which the indices are such that the product of the matrix elements on the right hand side of eqn. (6) is equal to unity.

To return to the constants C_{ijkl}, the relation

$$C_{ijkl} = \beta_{ip}\ \beta_{jq}\ \beta_{kr}\ \beta_{ls}\ \Gamma_{pqrs} \quad \ldots \quad (7)$$

may be used, where β is the inverse of α.

Application to Hexagonal and Trigonal Point Groups

Hexagonal System

Class $\bar{6}$ — In this case $\theta = 2\pi/6$, so that the non-zero Γ_{ijkl} are those for which the indices 1 and 2 appear equal number of times. Thus, there are only five non-zero elastic constants namely, Γ_{1122}, Γ_{1212}, Γ_{3312}, Γ_{2313} Γ_{3333}.

Class 6 — Addition of a centre of inversion to the class 6 will have no effect on the number of non-zero components since $\mathbf{A}'(\bar{1}) = \mathbf{A}(\bar{1})$. The number remains the same.

Class $6/m$ — The mirror plane perpendicular to the 6-fold axis (ox_3) transforms as

$$\mathbf{A}'(m_3) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}. \quad \ldots \quad (8)$$

The tensor components having even number of subscripts 3 are invariant under this transformation. The total non-zero constants will remain five.

Class 622 — The first 2-fold axis is along ox_1, which gives

$$\mathbf{A}'(2) = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}. \quad \dots (9)$$

The tensor components having even number of subscripts 3 and/or subscripts 1 and 2 symmetrical with each other remains invariant under this transformation.

The second 2-fold axis can be chosen along ox_2 (Nye, 1969) which in $0\ \xi_1\ \xi_2\ \xi_3$ system is

$$\mathbf{A}'(2') = \begin{pmatrix} 0 & \bar{1} & 0 \\ 1 & 0 & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}. \quad \dots (10)$$

With the same arguments, as stated above, the total number of constants are five.

Class : 6 mm — In this class, the first mirror plane is taken perpendicular to ox_1, which after transformation reduces to

$$\mathbf{A}'(m_1) = \begin{pmatrix} 0 & \bar{1} & 0 \\ \bar{1} & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}. \quad \dots (11)$$

The second mirror plane may be taken perpendicular to ox_2, so that

$$\mathbf{A}'(m_2) = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}. \quad \dots (12)$$

As the tensor components are symmetrical with respect to the subscripts 1 and 2, the total number of constants remain five.

Classes : $\bar{6}$ *m*2 *and* 6/*mmm* — The effects of the symmetry elements of these classes on the tensor components have already been considered and so there will not be any further reduction in the number of non-zero components.

Trigonal System

Class : 3 — In this case $\theta = 2\pi/3$, and in addition to five non-zero tensor components as in the previous case, there are two additional non-zero constants corresponding to the presence of indices 1 and 2 such that the difference between the number of times of their occurrence is 3. Hence the additional ones are Γ_{1113} and Γ_{2223}, giving the total number of non-zero independent components as seven.

Class : $\bar{3}$ — As in the case of class 3, in this case also the number of components will be seven since $\mathbf{A}'(\bar{1}) = \mathbf{A}(\bar{1})$.

Class : 32 — The operation of 2-fold rotation, according to eqn. (9) yields $\Gamma_{1113} = -\Gamma_{2223}$, so that the total number of independent constants is six.

Class : 3*m* — The operation of mirror, according to eqn. (11) gives $\Gamma_{1113} = -\Gamma_{2223}$. As in the case of class 32, total number remains six.

Class : $\bar{3}m$ — An addition of centre of inversion will not alter the total number of non-zero components and therefore the number remains six.

INDEPENDENT NON-ZERO COMPONENTS C_{ijkl}

The determination of independent non-zero components C_{ijkl} by expanding eqn. (7) is not very tedious due to small number of components Γ_{pqrs}. Also as β_{31} and β_{32} are zero the non-zero components C_{ijkl} have the same number of subscript 3 at the same position as in Γ_{pqrs} in eqn. (7). Following the method of expansion as given in Dieulesaint and Royer (1972), we obtain below the non-zero independent C_{ijkl} for hexagonal and trigonal systems.

Hexagonal system (*all classes*)

The component with four subscripts 3 is non-zero as

$$C_{3333} = \Gamma_{3333} \qquad \ldots (13)$$

The components with three subscripts 3, C_{3313} and C_{3323} are zero as Γ_{3313} and Γ_{3323} are zero.

The components with two subscripts 3, C_{ij33} and C_{i3k3} are expressed as functions of $\Gamma_{1233} = \Gamma_{2133}$ and $\Gamma_{1323} = \Gamma_{2313}$ respectively. These lead to

$$C_{1133} = C_{2233}, \quad C_{1233} = 0 \qquad \ldots (14)$$

and

$$C_{1313} = C_{2323}, \quad C_{2313} = 0 \qquad \ldots (15)$$

For hexagonal system, there are no non-zero Γs with one subscript 3, therefore there are no non-zero Cs with one subscript 3.

For components without subscript 3 expansion of eqn. (7) as functions of $\Gamma_{1122} = \Gamma_{2211}$ and $\Gamma_{1212} = \Gamma_{2112} = \Gamma_{2121}, = \Gamma_{1221}$, show

$$C_{1112} = C_{2212} = 0\,; \; C_{1111} = C_{2222}\,; \; C_{1212} = \tfrac{1}{2}(C_{1111} - C_{1122}) \qquad \ldots (16)$$

The relations (13) to (16) with two-suffix notation leads to five non-zero independent constants

$$C_{11} = C_{22}, \; C_{33}, \; C_{44}, = C_{55}, \; C_{66} = \tfrac{1}{2}(C_{11} - C_{12}),$$
$$C_{12}, \; C_{13} = C_{23}.$$

Trigonal system

Classes : 3 *and* $\bar{3}$ — For the point groups 3 and $\bar{3}$ belonging to the trigonal system two more components Γ_{1113} and Γ_{2223} appear. These are the components where subscript 3 appears only once. Therefore, from eqn. (7) one obtains

$$C_{22k3} = -C_{11k3} \text{ and } C_{i112} = -C_{i223} \qquad \ldots (17)$$

Eqn. (17) in turn leads in the two subscript form to

$$C_{14} = -C_{24} = C_{56} \text{ and } C_{15} = -C_{25} = -C_{46} \qquad \ldots (18)$$

Therefore, in this case, two extra components appear leading to a total number of seven non-zero components.

Classes : 32, $3m$ and $\bar{3}m$ — For the point groups 32, $3m$ and $\bar{3}m$ belonging to trigonal system, we have the further relation $\Gamma_{1113} = -\Gamma_{2223}$. Using eqn. (7), this gives the added relation

$$C_{15} = -C_{25} = -C_{46} = 0 \quad \dots \quad (19)$$

Therefore, in this case, one extra component in eqn. (18) disappears leaving six non-zero components.

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