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Fast Determination of the Number of Independent Tensor Components of Physical Properties of Crystals with *n*-Fold Axes of Symmetry ($n>2$)

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A method is outlined for determining in a simple way the number of independent tensor components of physical properties of crystals with an *n*-fold axis of symmetry, *n* being greater than 2. The procedure, which uses a change of axes to diagonalize the matrix of rotation, is illustrated in the case of the elastic tensor. The example of a trigonal crystal is given.

1. General case

It is known (Nye, 1957; Bhagavantam, 1966) that the symmetry of crystals reduces the number of independent tensor components, but the calculations are often tedious when the rank of the tensor is high. The tensor of the elastic moduli is chosen to illustrate the simple method we propose. For a crystal with an *n*-fold axis A_n ($n>2$), the condition for invariance of the elastic constants

$$C^{ijkl}=\beta^i_p\beta^j_q\beta^k_r\beta^l_s C^{pqrs} \tag{1}$$

is difficult to handle because the matrix $\boldsymbol{\beta}$ reciprocal to the rotation matrix $\boldsymbol{\alpha}$ is not diagonal. Let us set the axis A_n parallel to one of the axes, say Ox_3, of an orthonormalized coordinate system $Ox_1x_2x_3$:

$$\boldsymbol{\alpha}=\begin{pmatrix}\cos\varphi & \sin\varphi & 0\\ -\sin\varphi & \cos\varphi & 0\\ 0 & 0 & 1\end{pmatrix}\ \text{with}\ \varphi=\frac{2\pi}{n}. \tag{2}$$

The classical procedures (Fedorov, 1968) consist of developing equation (1) directly and give rise to tedious calculations. Only Landau & Lifchitz (1967) used a change of coordinates. Our method consists of expressing the relation of invariance in the eigenvector set of the rotation: $\xi_1(1,i,0)$; $\xi_2(i,1,0)$; $\xi_3(0,0,1)$, where i is the complex number ($i^2=-1$). As this new system is not orthogonal it is necessary to note that the elastic tensor is fourth order and contravariant according to the expression for energy density as a function of strain:

$$E=\tfrac{1}{2}C^{ijkl}S_{ij}S_{kl}\,. \tag{3}$$

The invariance relation for the new elastic moduli Γ^{ijkl} in the system $0\xi_1\xi_2\xi_3$ is a function of only the eigenvalues λ^i_i of the matrix $\boldsymbol{\beta}$:

$$\lambda^1_1=\exp -i\varphi;\ \lambda^2_2=\exp i\varphi;\ \lambda^3_3=1\,. \tag{4}$$

Thus, it is written as

$$\Gamma^{ijkl}=\lambda^i_i\lambda^j_j\lambda^k_k\lambda^l_l\Gamma^{ijkl}. \tag{5}$$

The only Γ^{ijkl} different from zero are those in which the difference between the number ν_1 of superscripts 1 and the number ν_2 of superscripts 2 is a multiple of the order n of the axis of symmetry, *i.e.* the product

$$\lambda^i_i\lambda^j_j\lambda^k_k\lambda^l_l=\exp\left[i\frac{2\pi}{n}(\nu_2-\nu_1)\right] \tag{6}$$

is equal to unity. Consequently, the number of independent elastic constants for crystals with an *n*-fold axis ($n>2$) immediately follows:

– five moduli Γ^{1122}, Γ^{1212}, Γ^{3312}, Γ^{2313}, Γ^{3333} such that $\nu_1=\nu_2$ are only possible for crystals of the hexagonal system ($n=6$);

– for the trigonal system ($n=3$), two other moduli Γ^{1113} and Γ^{2223} can exist ($\nu_2-\nu_1=\pm3$). Thus there are seven independent moduli;

– for the tetragonal system ($n=4$), two other different moduli are obtained, Γ^{1111} and Γ^{2222} ($\nu_2-\nu_1=\pm4$). This system also possesses seven independent moduli.

2. Example: The trigonal system

To return to the constants C^{ijkl}, relation (7) is used:

$$C^{ijkl}=\mathbf{b}^i_p\mathbf{b}^j_q\mathbf{b}^k_r\mathbf{b}^l_s\Gamma^{pqrs} \tag{7}$$

in which:

$$\mathbf{b}=\begin{pmatrix}1 & i & 0\\ i & 1 & 0\\ 0 & 0 & 1\end{pmatrix} \tag{8}$$

is the transition matrix from the old axis system $Ox_1x_2x_3$ to the eigenvector set $\xi_1\xi_2\xi_3$. The expansion of relation (7) is easy, due to the low number of components Γ^{pqrs}. Moreover, the coefficients b_1^3 and b_2^3 are zero so that the only constants found have the same order of superscripts 3 as the i, j, k, l set. For example, let us consider the case of the trigonal system.

– Clearly

$$C^{3333} = \Gamma^{3333}. \tag{9}$$

– The moduli with three superscripts 3 (C^{3313} and C^{3323}) are zero because $\Gamma^{3313} = \Gamma^{3323} = 0$.

– The moduli with two superscripts 3 (C^{ij33} and C^{i3k3}) are expressed as a function of $\Gamma^{1233} = \Gamma^{2133}$ and $\Gamma^{1323} = \Gamma^{2313}$:

$$C^{ij33} = (b_1^i b_2^j + b_2^i b_1^j)\Gamma^{1233}. \tag{10}$$

It follows that:

$$C^{1133} = C^{2233} \tag{11}$$

and as

$$b_1^1 b_2^2 + b_2^1 b_1^2 = 0,$$
$$C^{1233} = 0. \tag{12}$$

Similarly the relation:

$$C^{i3k3} = (b_1^i b_2^k + b_2^i b_1^k)\Gamma^{1323} \tag{13}$$

leads to:

$$C^{2313} = 0 \quad \text{and} \quad C^{1313} = C^{2323}. \tag{14}$$

– For the moduli with only one superscript 3:

$$C^{ijk3} = b_1^i b_1^j b_1^k \Gamma^{1113} + b_2^i b_2^j b_2^k \Gamma^{2223} \tag{15}$$

as

$$b_1^1 b_1^1 = b_2^2 b_2^2 = -b_1^2 b_1^2 = -b_2^1 b_2^1 . \tag{16}$$

It follows that

$$C^{22k3} = -C^{11k3} \quad \text{and} \quad C^{i113} = -C^{i223} \tag{17}$$

or, using the more concise form with two superscripts:

$$C^{14} = -C^{24} = C^{56} \quad \text{and} \quad C^{15} = -C^{25} = C^{46}. \tag{18}$$

– The relation (7) applied to moduli without superscripts 3 shows that:

$$C^{1112} = C^{2212} = 0 \quad \text{and} \quad C^{1111} = C^{2222}. \tag{19}$$

This results lead to the eight non-zero moduli

$$C^{33};\ C^{13};\ C^{44};\ C^{14};\ C^{15};\ C^{11};\ C^{12};\ C^{66}.$$

Since we have stated that only 7 elastic constants are independent, there must be a relation among these moduli. Examining C^{11}, C^{12} and C^{66} it is found that:

$$C^{66} = \frac{C^{11} - C^{12}}{2}. \tag{20}$$

Table 1 presents the results for crystals of the trigonal system with the axis of symmetry parallel to the Ox_3 axis.

Table 1. *Elastic constants for a crystal of the trigonal system with the θ symmetry axis parallel to the Ox_3 axis*

C^{11}	C^{12}	C^{13}	C^{14}	C^{15}	0
C^{12}	C^{11}	C^{13}	$-C^{14}$	$-C^{15}$	0
C^{13}	C^{13}	C^{33}	0	0	0
C^{14}	$-C^{14}$	0	C^{44}	0	$-C^{15}$
C^{15}	$-C^{15}$	0	0	C^{44}	C^{14}
0	0	0	$-C^{15}$	C^{14}	$\frac{C^{11}-C^{12}}{2}$

The method developed here for the elastic tensor is suitable for a tensor of any rank.

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