Note on sufficient symmetry conditions for isotropy of the elastic moduli tensor

M. S. Dresselhaus
Department of Electrical Engineering and Computer Science and Department of Physics, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139

G. Dresselhaus
Francis Bitter National Magnet Laboratory, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139

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Group theoretical methods are used to obtain the form of the elastic moduli matrices and the number of independent parameters for various symmetries. Particular attention is given to symmetry groups for which 3D and 2D isotropy is found for the stress-strain tensor relation. The number of independent parameters is given by the number of times the fully symmetric representation is contained in the direct product of the irreducible representations for two symmetrical second rank tensors. The basis functions for the lower symmetry groups are found from the compatibility relations and are explicitly related to the elastic moduli. These types of symmetry arguments should be generally useful in treating the elastic properties of solids and composites.

I. INTRODUCTION

Christensen has shown[1] that the 4th rank symmetric elastic tensor C_{ijkl} defined by

$$\frac{\partial F_i}{\partial r_j} = \sum_{k,l=x,y,z} C_{ijkl} e_{kl} \tag{1}$$

where F_i is the component of the force in direction r_j, retains its form in three dimensions (3D) in going from the isotropic full rotational symmetry group to the case of 6 fivefold axes. Christensen further obtained the corresponding result in two dimensions (2D) where the form of the C_{ijkl} is retained in going from the case of full axial symmetry (in-plane isotropy) to hexagonal symmetry with a sixfold axis. In his paper Christensen[1] emphasizes that the more restricted symmetry of the 6 fivefold axes in the 3D case and the hexagonal axis in the 2D case is sufficient to yield 3D and 2D isotropy with regard to the elastic properties, defined by Eq. (1).

Fiber reinforced composites represent an interesting application of these symmetry forms.[1] If the fibers are oriented in three dimensional space in the six directions prescribed by icosahedral symmetry, then isotropy of the elastic moduli tensor will be obtained. This possibility was first suggested by Rosen.[2] In the corresponding two dimensional situation, if the fibers are oriented at 60° intervals, then isotropy is obtained in the plane. It is standard practice to use fiber composite sheets stacked at 60° angular intervals to obtain "quasi-isotropy" in the field of fiber composites. Recent research on quasicrystals[3,4] has emphasized the connection of the icosahedral symmetry to the elastic properties.[3,4]

In this note we show a generalization of Christensen's proof, using group theoretical arguments. From the group theoretical point of view presented here, the conditions for retaining isotropy can be clearly defined and when the symmetry is further lowered to introduce anisotropy in the elastic properties, the passage from the isotropic to the anisotropic situations can be followed adiabatically through use of compatibility relations. For those with a group theory background, the results of this note are almost obvious, but for materials scientists without this background, these results do not seem so obvious. The objective of this note, then, is to make certain symmetry results available to materials scientists for use in their applications.

II. 3D ISOTROPY

For the case of full rotational symmetry, a second rank tensor $\overleftrightarrow{T}$ transforms according to the representation $\Gamma_{\overleftrightarrow{T}}$ where $\Gamma_{\overleftrightarrow{T}}$ can be written as a symmetric and an antisymmetric part

$$\Gamma_{\overleftrightarrow{T}} = \Gamma_{\overleftrightarrow{T}}^{(s)} + \Gamma_{\overleftrightarrow{T}}^{(a)} \tag{2}$$

where the symmetric components transform as the irreducible representations

$$\Gamma_{\overleftrightarrow{T}}^{(s)} = \Gamma_{l=0} + \Gamma_{l=2} \tag{3}$$

and the antisymmetric components transform as

$$\Gamma_{\overleftrightarrow{T}}^{(a)} = \Gamma_{l=1}, \tag{4}$$

in which the irreducible representations of the full rotation group are denoted by their total angular momentum values l. Since the stress $\vec{\nabla} \cdot \overleftrightarrow{F}$ and strain $\overleftrightarrow{e}$ tensors are symmetric second rank tensors, both X_α and e_{ij} transform according to $(\Gamma_{l=0} + \Gamma_{l=2})$ in full rotational symmetry, where X_α denotes a force in the x direction applied to a plane whose normal is in the α direction. The fourth rank symmetric C_{ijkl} tensor of Eq. (1) transforms according to the symmetric part of the direct product of two second rank symmetric tensors $\Gamma_e^{(s)} \otimes \Gamma_e^{(s)}$ yielding

$$(\Gamma_{l=0} + \Gamma_{l=2}) \otimes (\Gamma_{l=0} + \Gamma_{l=2}) = (2\Gamma_{l=0} + 2\Gamma_{l=2} + \Gamma_{l=4})^{(s)} + (\Gamma_{l=1} + \Gamma_{l=2} + \Gamma_{l=3})^{(a)}, \quad (5)$$

so that in general e_{ij} is specified by 6 constants and the C_{ijkl} tensor by 21 constants because it is symmetrical under the interchange of $ij \leftrightarrow kl$. The additional 15 constants that specify the antisymmetric off-diagonal irreducible representations are not needed to specify the C_{ijkl}. In the case of full rotational symmetry, Eq. (5) shows that the totally symmetric representation ($\Gamma_{l=0}$) is contained only twice in the direct product of the irreducible representations for two second rank symmetric tensors, indicating that only two independent nonvanishing constants are needed to describe the 21 constants of the C_{ijkl} tensor, a result that is well known in elasticity theory for isotropic media. In general, the number of times the totally symmetric representation (e.g., $\Gamma_{l=0}$ for the full rotational group) is contained in the irreducible representations of a general matrix of arbitrary rank gives the number of independent nonvanishing constants needed to specify that matrix.

We denote the two independent nonvanishing constants needed to specify the C_{ijkl} tensor by C_0 for $\Gamma_{l=0}$ and by C_2 for $\Gamma_{l=2}$ symmetry. We then use these two constants to relate symmetrized stresses and strains labeled by the irreducible representations $\Gamma_{l=0}$ and $\Gamma_{l=2}$ in the full rotation group. The symmetrized stress-strain equations are first written in full rotational symmetry, using the partners of the irreducible representations (one for $l = 0$ and five for the $l = 2$ partners):

$$(X_x + Y_y + Z_z) = C_0(e_{xx} + e_{yy} + e_{zz}) \quad \text{for } l = 0, m = 0$$

$$(X_x - Y_y + iY_x + iX_y) = C_2(e_{xx} - e_{yy} + ie_{xy} + ie_{yx}) \quad \text{for } l = 2, m = 2$$

$$(Z_x + X_z + iY_z + iZ_y) = C_2(e_{zx} + e_{xz} + ie_{yz} + ie_{zy}) \quad \text{for } l = 2, m = 1$$

$$\left[Z_z - \frac{1}{2}(X_x + Y_y)\right] = C_2\left[e_{zz} - \frac{1}{2}(e_{xx} + e_{yy})\right] \quad \text{for } l = 2, m = 0$$

$$(Z_x + X_z - iY_z - iZ_y) = C_2(e_{zx} + e_{xz} - ie_{yz} - ie_{zy}) \quad \text{for } l = 2, m = -1$$

$$(X_x - Y_y - iY_x - iX_y) = C_2(e_{xx} - e_{yy} - ie_{xy} - ie_{yx}) \quad \text{for } l = 2, m = -2 \quad (6)$$

From Eq. (6) we solve for the six independent stress coefficients in terms of the strains, yielding

$$X_x = \left(\frac{C_0}{3} + \frac{2C_2}{3}\right)e_{xx} + \left(\frac{C_0}{3} - \frac{C_2}{3}\right)(e_{yy} + e_{zz}) \quad (7)$$

for the stress component X_x. Five additional relations are then written down for the other five stress components.

In the notation that is commonly used, we write the stress-strain relations

$$\sigma_i = \sum_{j=1,6} C_{ij}\epsilon_j, \quad (8)$$

where the six components of the symmetric stress and strain tensors are written as

$$\sigma_1 = X_x \qquad \epsilon_1 = e_{xx}$$

$$\sigma_2 = Y_y \qquad \epsilon_2 = e_{yy}$$

$$\sigma_3 = Z_z \qquad \epsilon_3 = e_{zz}$$

and

$$\sigma_4 = \frac{1}{2}(Y_z + Z_y) \qquad \epsilon_4 = (e_{yz} + e_{zy})$$

$$\sigma_5 = \frac{1}{2}(Z_x + X_z) \qquad \epsilon_5 = (e_{zx} + e_{xz})$$

$$\sigma_6 = \frac{1}{2}(X_y + Y_x) \qquad \epsilon_6 = (e_{xy} + e_{yx}) \quad (9)$$

and C_{ij} is the 6×6 elastic moduli matrix C_{ij}. In this notation the 21 partners that transform as $(2\Gamma_{l=0} + 2\Gamma_{l=2} + \Gamma_{l=4})$ in Eq. (5) correspond to the symmetric partners while the 15 partners in $(\Gamma_{l=1} + \Gamma_{l=2} + \Gamma_{l=3})$ correspond to the antisymmetric partners that do not give rise to any independent elastic components, since $C_{ij} = C_{ji}$. From the six relations for the six stress components [one of which is given explicitly by Eq. (7)], the relations among the C_0 and C_2 and the C_{ij} follow:

$$C_{11} = \frac{1}{3}(C_0 + 2C_2) = C_{22} = C_{33}$$

$$C_{12} = \frac{1}{3}(C_0 - C_2) = C_{13} = C_{23}$$

$$C_{44} = \frac{1}{2}C_2 = C_{55} = C_{66} \quad (10)$$

from which we construct the C_{ij} matrix for a 3D isotropic medium involving two independent constants C_{11} and C_{12}

$$C_{ij} = \begin{bmatrix} C_{11} & C_{12} & C_{12} & 0 & 0 & 0 \\ & C_{11} & C_{12} & 0 & 0 & 0 \\ & & C_{11} & 0 & 0 & 0 \\ & & & \frac{1}{2}(C_{11} - C_{12}) & 0 & 0 \\ & & & & \frac{1}{2}(C_{11} - C_{12}) & 0 \\ & & & & & \frac{1}{2}(C_{11} - C_{12}) \end{bmatrix} \tag{11}$$

Any subgroup of the full rotation group for which the fivefold $\Gamma_{l=2}$ level degeneracy is not lifted will leave the form of the C_{ij} matrix invariant, thus giving a more general proof of Christensen's arguments.[1] The icosahedral group with inversion symmetry I_h, which is a subgroup of the full rotation group, and the icosahedral group without inversion I, which is a subgroup of both the full rotation group and the group I_h, are two examples of groups which preserve the fivefold degenerate level and hence retain the form of the C_{ij} matrix given by Eq. (11). This result follows from at least two related arguments. Firstly, from the pertinent compatibility relations between the full rotation group[5,6] and the I_h group (see Table I for the character table; note that since Refs. 5 and 6 and other standard references do not list the character tables for the icosahedral groups I and I_h, we have included a character table for the group I_h)

$$\Gamma_{l=0} \rightarrow (A_g)_{I_h}$$
$$\Gamma_{l=2} \rightarrow (H_g)_{I_h} \tag{12}$$

we show that

$$\Gamma^{(s)}_{\overleftrightarrow{e}} = (A_g)_{I_h} + (H_g)_{I_h} . \tag{13}$$

From Eq. (13) we see that no lifting of degeneracy occurs in going from full rotational symmetry to I_h symmetry from which it follows that the number of nonvanishing independent constants in the C_{ij} matrix remains at 2 for I_h (and I) symmetry.

The same conclusion follows from the fact that the basis functions for $\Gamma_{l=0}$ and $\Gamma_{l=2}$ for the full rotation group can also be used as basis functions for the A_g and H_g irreducible representations of I_h. Therefore the same stress-strain relations are obtained in I_h symmetry as are given in Eq. (6). It therefore follows that the form of the C_{ij} matrix will also be the same for I_h and full rotational symmetry, thereby completing the proof.

Clearly, the direct product $\Gamma^{(s)}_{\overleftrightarrow{e}} \otimes \Gamma^{(s)}_{\overleftrightarrow{e}}$ given by Eq. (5) is not invariant as the symmetry is reduced from full rotational symmetry to I_h symmetry since the ninefold representation $\Gamma_{l=4}$ in Eq. (5) splits into the irreducible representations $(G_g + H_g)$ in going to the lower symmetry group I_h. But this is not of importance to the linear stress-strain equations which are invariant to this lowering of symmetry. It might be worth mentioning here that when nonlinear effects are taken into account and perturbations from Eq. (1) are needed to specify the stress-strain relations (for example, terms in the strain squared), different mechanical behavior would be expected to occur in I_h symmetry in comparison with the full rotation group. In such a case, the compatibility relations between the full rotation group and the I_h group [e.g., Eq. (12)] can be used to relate the terms in the generalized elastic moduli matrix for the two symmetries.

It should be noted that all symmetry groups forming Bravais lattices in solid state physics have too few symmetry operations to preserve the fivefold degeneracy of the $l = 2$ level; for example, in cubic O_h symmetry, the cubic group with the highest symmetry, the $l = 2$ level corresponds to a reducible representation of group O_h, which splits into a threefold and a twofold level (the T_{2g} and E_g levels), so that in this case [see Eq. (6)], three elastic constants are needed to specify the 6×6 matrix for C_{ij}

$$C_{ij} = \begin{bmatrix} C_{11} & C_{12} & C_{12} & 0 & 0 & 0 \\ & C_{11} & C_{12} & 0 & 0 & 0 \\ & & C_{11} & 0 & 0 & 0 \\ & & & C_{44} & 0 & 0 \\ & & & & C_{44} & 0 \\ & & & & & C_{44} \end{bmatrix} \tag{14}$$

as is described in many solid state physics books.[7,8]

III. 2D ISOTROPY

A similar situation applies in 2D. Here the full axial symmetry is described by the group $D_{\infty h}$. The irreducible representations of $D_{\infty h}$ that are contained in the symmetric second rank tensor are

$$\Gamma^{(s)}_{\overleftrightarrow{e}} = 2A_{1g} + E_{1g} + E_{2g} \tag{15}$$

so that the symmetric part of the direct product becomes

$$(\Gamma^{(s)}_{\overleftrightarrow{e}} \otimes \Gamma^{(s)}_{\overleftrightarrow{e}})^{(s)} = 5A_{1g} + 3E_{1g} + 3E_{2g} + E_{3g} + E_{4g} , \tag{16}$$

indicating that the C_{ij} matrix can be described in terms of five independent constants for full axial symmetry. The stress-strain relations for $D_{\infty h}$ symmetry are writ-

TABLE I. Character table for I_h.

I_h	E	$12C_5$	$12C_5^2$	$20C_3$	$15C_2$	i	$12S_{10}$	$12S_{10}^3$	$20S_{10}$	15σ	Basis functions
A_g	1	1	1	1	1	1	1	1	1	1	$x^2 + y^2 + z^2$
F_{1g}	3	τ	$1-\tau$	0	-1	3	$1-\tau$	τ	0	-1	R_x, R_y, R_z
F_{2g}	3	$1-\tau$	τ	0	-1	3	τ	$1-\tau$	0	-1	
G_g	4	-1	-1	1	0	4	-1	-1	1	0	
H_g	5	0	0	-1	1	5	0	0	-1	1	$\{2z^2 - x^2 - y^2$, $x^2 - y^2$, xy, xz, yz
A_u	1	1	1	1	1	-1	-1	-1	-1	-1	
F_{1u}	3	τ	$1-\tau$	0	-1	-3	$\tau-1$	$-\tau$	0	1	(x, y, z)
F_{2u}	3	$1-\tau$	τ	0	-1	-3	$-\tau$	$\tau-1$	0	1	(x^3, y^3, z^3)
G_u	4	-1	-1	1	0	-4	1	1	-1	0	$\{x(z^2 - y^2)$, $y(z^2 - x^2)$, $z(x^2 - y^2)$, xyz
H_u	5	0	0	-1	1	-5	0	0	1	-1	

where $\tau = (1 + \sqrt{5})/2$ and is often referred to as the "golden mean".

ten in symmetrized form using the basis functions

$$(X_x + Y_y + Z_z) \quad \text{and} \quad (e_{xx} + e_{yy} + e_{zz})$$
$$\text{for } l = 0,\ m = 0 \text{ and symmetry } A_{1g}$$
$$(X_x - Y_y + iY_x + iX_y) \quad \text{and} \quad (e_{xx} - e_{yy} + ie_{xy} + ie_{yx})$$
$$\text{for } l = 2,\ m = 2 \text{ and symmetry } E_{2g}$$
$$(X_x - Y_y - iY_x - iX_y) \quad \text{and} \quad (e_{xx} - e_{yy} - ie_{xy} - ie_{yx})$$
$$\text{for } l = 2,\ m = -2 \text{ and symmetry } E_{2g}$$
$$(Z_x + X_z + iY_z + iZ_y) \quad \text{and} \quad (e_{zx} + e_{xz} + ie_{yz} + ie_{zy})$$
$$\text{for } l = 2,\ m = 1 \text{ and symmetry } E_{1g}$$
$$(Z_x + X_z - iY_z - iZ_y) \quad \text{and} \quad (e_{zx} + e_{xz} - ie_{yz} - ie_{zy})$$
$$\text{for } l = 2,\ m = -1 \text{ and symmetry } E_{1g}$$
$$\left[Z_z - \frac{1}{2}(X_x + Y_y)\right] \quad \text{and} \quad \left[e_{zz} - \frac{1}{2}(e_{xx} + e_{yy})\right]$$
$$\text{for } l = 2,\ m = 0 \text{ and symmetry } A_{1g} \tag{17}$$

yielding

$$X_x + Y_y + Z_z = C_{A_{1g},1}(e_{xx} + e_{yy} + e_{zz}) + C_{A_{1g},3}\left[e_{zz} - \frac{1}{2}(e_{xx} + e_{yy})\right]$$
$$Z_z - \frac{1}{2}(X_x + Y_y) = C_{A_{1g},2}\left[e_{zz} - \frac{1}{2}(e_{xx} + e_{yy})\right] + C_{A_{1g},4}[e_{xx} + e_{yy} + e_{zz}]$$
$$X_x - Y_y = C_{E_{2g}}(e_{xx} - e_{yy}) \tag{18}$$

and corresponding equations for X_y, Y_z, and Z_x. We then solve Eqs. (18) for X_x, Y_y, and Z_z and require $C_{ij} = C_{ji}$.

In the case of $D_{\infty h}$, the requirement that $C_{31} = C_{13} = C_{32} = C_{23}$ yields the additional constraint $C_{A_{1g},3} = 2C_{A_{1g},4}$ which is needed to obtain the five independent symmetry coefficients as required by Eq. (16): $C_{A_{1g},1}$, $C_{A_{1g},2}$, $C_{A_{1g},3}$, $C_{E_{1g}}$, and $C_{E_{2g}}$. The relations between these symmetry coefficients and the C_{ij} coefficients are:

$$C_{11} = C_{22} = \frac{1}{2}\left[\frac{2}{3}C_{A_{1g},1} + \frac{1}{3}C_{A_{1g},2} - \frac{2}{3}C_{A_{1g},3} + C_{E_{2g}}\right]$$
$$C_{12} = C_{21} = \frac{1}{2}\left[\frac{2}{3}C_{A_{1g},1} + \frac{1}{3}C_{A_{1g},2} - \frac{2}{3}C_{A_{1g},3} - C_{E_{2g}}\right]$$
$$C_{13} = C_{23} = \frac{1}{3}\left[C_{A_{1g},1} - C_{A_{1g},2} + \frac{1}{2}C_{A_{1g},3}\right]$$
$$C_{33} = \frac{1}{3}[C_{A_{1g},1} + 2C_{A_{1g},2} + 2C_{A_{1g},3}]$$
$$C_{44} = C_{55} = \frac{1}{2}C_{E_{1g}}$$
$$C_{66} = \frac{1}{2}C_{E_{2g}} = \frac{1}{2}(C_{22} - C_{21}) = \frac{1}{2}(C_{11} - C_{12}). \tag{19}$$

Combining the nonvanishing C_{ij} coefficients then yields the C_{ij} matrix for full axial symmetry $D_{\infty h}$

$$C_{ij} = \begin{bmatrix} C_{11} & C_{12} & C_{13} & 0 & 0 & 0 \\ & C_{11} & C_{13} & 0 & 0 & 0 \\ & & C_{33} & 0 & 0 & 0 \\ & & & C_{44} & 0 & 0 \\ & & & & C_{44} & 0 \\ & & & & & \frac{1}{2}(C_{11} - C_{12}) \end{bmatrix}. \quad (20)$$

Once again, the basis functions used to obtain the stress-strain relations also serve as a basis functions for the irreducible representations A_{1g}, E_{1g}, and E_{2g} in the hexagonal group D_{6h}, although D_{6h} is not a subgroup of $D_{\infty h}$. Thus the stress-strain relations for D_{6h} symmetry are identical to $D_{\infty h}$ and the same form of the 6×6 C_{ij} matrix follows, completing a generalization of the result proven by Christensen in 2D.[1]

If we consider the axial group with the next highest symmetry (D_{4h}), we immediately see that there is only one 2-dimensional irreducible representation[5,6] in D_{4h} so that the irreducible representations contained in second rank tensor $\Gamma_{\overleftrightarrow{\epsilon}}$ are not invariant as the symmetry is reduced from full axial symmetry to D_{4h}.

It must be emphasized that in going from full rotational symmetry to I_h symmetry or in going from $D_{\infty h}$ to D_{6h}, the number of symmetry operations goes from ∞ to a relatively small number (120 for I_h and 24 for D_{6h}), so that some relations involving tensors of rank higher than 2 (such as the electrooptic coefficients) are no longer invariant under this lowering of symmetry both in 3D and in 2D.

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