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Invariants of 3D Anisotropic Elasticity Tensor: Measure of Symmetry Defects

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Abstract Hooke's Law Formula is given as $F = -kx$, where F denotes the force applied, x is the displacement extension and k is the spring constant or force constant. In classical linear elasticity, with the stress tensor σ and the strain tensor ε, the generalized Hooke's law is written: $\sigma_{ij} = C_{ijkl}\varepsilon_{kl}$, where the tensor of fourth order $C = \left(C_{ijkl}\right)$ is called tensor of elasticity. It is a tensor generalization of the stiffness constant k of a spring. The invariants of the elasticity tensors represent mechanical characteristics of the anisotropic materials (such as elasticity, ductility, resistance to deformations), help to classify materials following their symmetries, which generalize the concept of "stiffness of a spring". In this paper, we perform the calculation of invariants for the anisotropic elasticity tensor under the rotation action of SO(3) groups. The tools developed by G. de Saxé et al. [1] to determine the independent invariants in 2D, essentially consisting of changing reference base and Kelvin's decomposition of the elasticity tensor, are borrowed for the 3D case. In total, eighteen independent invariants also called global invariant emerge including 5 for the first order and thirteen for higher order. At the end, we give the physical signification of these invariants for isotropic materials.

Keywords: *Representation theory, Anisotropy, Linear elasticity*

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1. Introduction

The elasticity tensor is a fourth-rank tensor describing the stress-strain relation in a linear elastic body (Cowin [2] and Hehl [3]). For the constitutive law in linear elasticity for a homogeneous anisotropic body, the generalized Hooke's law postulates a linear relation between the second-rank tensor field stress σ_{ij} and the second-rank tensor strain ε_{kl} :

$$\sigma_{ij} = C_{ijkl}\varepsilon_{kl} \tag{1}$$

The components of C generally acquire different values under a change of basis. Nevertheless, for certain types of transformations, there are specific combinations of components, called invariants, that remain unchanged. Invariants are defined concerning a given set of transformations formally known as a group operation. For example, an invariant for the group of proper orthogonal transformations called SO(3), is a quantity that remains constant under arbitrary 3D rotations.

In mechanics, the search for the invariants is essential. It is used for materials geometry reconstitution and for mechanical properties determination. Some authors (Olive et al. [4], Ahmad [5], Norris [6], Thomson et al. [7], Ting [8], Thomson [9], Boehler [10]) developed methods for determining elasticity tensor invariants in 3D, but not explicitly the independent invariants allowing the measurement of symmetry defects.

Thanks to Forte et al. [11], it's known that there are eight classes of three-dimensional symmetries (with eighteen corresponding invariants according to de Saxé). Currently, a finite base of invariants allowing identification of the class of materials in 2D is known thanks to the works of G. de Saxé [1], Auffray et al. [12] and Atchonouglo et al. [13].

Concerning the 3D case, G. de Saxé predicted eighteen independent invariants that engineers should take into consideration when measuring symmetry defects in materials. Certainly, an integrity base of 299 invariants was proposed by Olive et al. [4] but it turned out that these were not minimal at the end of Olive's work in 2017 [14]. It was corrected in 2019 by Olive et al. [15], who reported 297 invariants instead of 299. All these invariants do not yet allow the measurement of symmetry defects in materials or the explicit classification of materials according to the eighteen symmetry classes. They [14,15] also talk about global invariants which would be eighteen hesitating about their existence.

Curiously, until now no one has been interested in these eighteen invariants in the literature.

In this paper, we will try to prove their existence and see their application in measuring symmetry defects in the case of isotropic materials. We use tools developed by G. de Saxé et al. [1] consisting in Kelvin's representation [7] and a decomposition of elasticity tensor in irreducible under the action of element of SO(3).

First, in the subsections of section 3, we adapt the tools proposed by G. de Saxé et al. [1], in their works in two dimensions for the three-dimensional case with a rotation matrix around the z-axis. Second, Kelvin's representation under the generalized form is used to parameterize the stress tensor. This allows us to define an action that acts on the elasticity tensor. This action was performed by Ting using an orthogonal matrix Q. Then, Ting decomposes the new elasticity tensor into six groups. For our approach, the orthogonal matrix Q is a rotational matrix R and the elasticity tensor due to Kelvin's representation is decomposed into four groups. The five linear invariants determined by Ting and Ahmad, were obtained. For the second-order and third-order invariants, some of them are in the literature.

In the last section, we discuss the measurement of symmetry defects of isotropic materials.

2. Methodology

The approach used to determine the invariants by acting an element of SO(3) on the elasticity tensor is described in this section.

2.1. Hooke's Law and Kelvin's Representation

The orbits of elasticity tensor space $S^2S^2R^3$ under the action of **SO(3)** on R^3 are described by E when for linear representation

$$C' = \rho(r)C$$

where

$$E = \{C' \in E(3) | \exists r \in SO(3), C' = \rho(r)C\}$$

In classical linear elasticity, Hooke's law states that $\sigma = C\varepsilon$. This law can be represented by Voigt's representation and Kelvin's one. But Voigt's notation is not relevant for an easy study of symmetries. We will then use Kelvin's representation (Thomson et al. [7], Thomson [9]) where C expression is:

$$\begin{bmatrix} C_{1111} & C_{1122} & C_{1133} & \sqrt{2}C_{1123} & \sqrt{2}C_{1113} & \sqrt{2}C_{1112} \\ C_{1122} & C_{2222} & C_{2233} & \sqrt{2}C_{2223} & \sqrt{2}C_{2213} & \sqrt{2}C_{2212} \\ C_{1133} & C_{3322} & C_{3333} & \sqrt{2}C_{3323} & \sqrt{2}C_{3313} & \sqrt{2}C_{3312} \\ \sqrt{2}C_{2311} & \sqrt{2}C_{2322} & \sqrt{2}C_{2333} & 2C_{2323} & 2C_{2313} & 2C_{2312} \\ \sqrt{2}C_{1311} & \sqrt{2}C_{1322} & \sqrt{2}C_{1333} & 2C_{1323} & 2C_{1313} & 2C_{1312} \\ \sqrt{2}C_{1211} & \sqrt{2}C_{1222} & \sqrt{2}C_{1233} & 2C_{1223} & 2C_{1213} & 2C_{1212} \end{bmatrix} \quad (2)$$

using Kelvin's representation and changing the notation of stress tensor σ to s we can have the following generalized form:

$$\begin{cases} s_{ij} = \sigma_{ij} \; for \; i = 1,2,3,\ldots,d \\ s_{\left(3+\frac{d(d+1)}{2}-(i+j)\right)} = \sqrt{2}\sigma_{ij} \; for \; i,j = 1,2,3,\ldots,d, with \; i < j \end{cases} \quad (3)$$

thus for $d=3$ we have:

$$s_1' = \sigma_{11}'; s_2' = \sigma_{22}'; s_3' = \sigma_{33}'; s_4' = \sigma_{23}';$$
$$s_5' = \sigma_{13}'; s_6' = \sigma_{12}'$$

2.2. Parameterization of the Stress Tensor

We apply a rotation of angle θ on the stress tensor along the Z axis in dimension three. According to Monteghetti [16] and Euler [17], the rotation matrix r_θ is:

$$r_\theta = \begin{pmatrix} cos\theta & sin\theta & 0 \\ -sin\theta & cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad (4)$$

let's write $\sigma' = r_\theta^t \sigma r_\theta$, we can write $\sigma' = R'\sigma$ with:

$$R' = \begin{pmatrix} \cos^2\theta & \sin^2\theta & 0 & 0 & 0 & 2sin\theta cos\theta \\ \sin^2\theta & \cos^2\theta & 0 & 0 & 0 & -2sin\theta cos\theta \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & cos\theta & -sin\theta & 0 \\ 0 & 0 & 0 & sin\theta & cos\theta & 0 \\ -sin\theta cos\theta & sin\theta cos\theta & 0 & 0 & 0 & \cos^2\theta - \sin^2\theta \end{pmatrix} \quad (5)$$

Considering the relation (2) in the same way, we have:

$$s_1' = \sigma_{11}'; s_2' = \sigma_{22}'; s_3' = \sigma_{33}'; s_4' = \sigma_{23}';$$
$$s_5' = \sigma_{13}'; s_6' = \sigma_{12}'$$

The elements of ***S'*** are then given by:

$$\begin{cases} s_1' = \sigma_{11}' = s_1\cos^2\theta + \sqrt{2}s_6 cos\theta sin\theta + s_2\sin^2\theta \\ s_2' = \sigma_{22}' = s_1\sin^2\theta - \sqrt{2}s_6 cos\theta sin\theta + s_2\cos^2\theta \\ s_3' = \sigma_{33}' = s_3 \\ s_4' = \sqrt{2}\sigma_{23}' = s_4 cos\theta - s_5 sin\theta \\ s_5' = \sqrt{2}\sigma_{13}' = s_4 sin\theta + s_5 cos\theta \\ s_6' = \sqrt{2}\sigma_{12}' \\ s_6' = -\sqrt{2}(s_4 - s_5)cos\theta sin\theta + s_6(\cos^2\theta - \sin^2\theta) \end{cases} \quad (6)$$

as a function of θ. Wich leads to (7) where elements of ***s'*** are a function of θ and 2θ:

$$\begin{cases} s_1' = \frac{s_1+s_2}{2} + \frac{s_1-s_2}{2}\cos 2\theta + \frac{s_6}{\sqrt{2}}\sin 2\theta \\ s_2' = \frac{s_1+s_2}{2} - \frac{s_1-s_2}{2}\cos 2\theta - \frac{s_6}{\sqrt{2}}\sin 2\theta \\ s_3' = s_3 \\ s_4' = s_4\cos\theta - s_5\sin\theta \\ s_5' = s_4\sin\theta + s_5\cos\theta \\ s_6' = \frac{-1}{\sqrt{2}}(s_1-s_2)\sin 2\theta + s_6\cos 2\theta \end{cases} \quad (7)$$

It is then suggested to use the following parameters in the old and new orthogonal frame:

$$\begin{cases} p = \frac{s_1+s_2}{\sqrt{2}}; k = \frac{s_1-s_2}{\sqrt{2}} \\ p' = \frac{s_1'+s_2'}{\sqrt{2}}; k' = \frac{s_1'-s_2'}{\sqrt{2}} \end{cases} \quad (8)$$

We make some permutations and pass to $s(s_1, s_2, s_3, s_5, s_6)$ into $s^*(p,k,s_6,s_4,s_5,s_3)$, a new base formed by $(e_1,e_2,e_6,e_4,e_5,e_3)$.

$$s^* = Ps \quad (9)$$

In this new base, the elements of s' are given by $s^{*'} = Rs^*$ with R:

$$R = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & \cos 2\theta & \sin 2\theta & 0 & 0 & 0 \\ 0 & -\sin 2\theta & \cos 2\theta & 0 & 0 & 0 \\ 0 & 0 & 0 & cos\theta & -sin\theta & 0 \\ 0 & 0 & 0 & sin\theta & cos\theta & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix} \quad (10)$$

Along the e_1 axis we have one invariant (*p*), (s_3) along e_6 axis, $(q_1)^2$ formed by e_2 and e_3 and $(q_2)^2$ formed by e_4 and e_5. The first two represent straight lines and the last two describe Mohr circles with radius q_1 and $(1/\sqrt{2})q_2$ respectively.

We also verify that R is a rotation matrix: det(R) = 1 and $R^t = R$.

It is this rotation matrix R that we will use in the following lines.

2.3. Permutations and Decomposition of the Elasticity Tensor

By analogy to Kelvin's representation, we set $C_{IJ} = C_{ijkl}$. Considering the permutations performed in (7) we rewrite C according to Hooke's law:

$$s = Ce$$

With s the stress tensor, C the elasticity and e for strain tensor. From the equation (8) we deduced

$$C^* = P^{-1}CP \quad (11)$$

where:

$$P = P^{-1} = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 & 0 & 0 & 0 \\ \frac{1}{\sqrt{2}} & \frac{-1}{\sqrt{2}} & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

We get the new elasticity tensor that we note C***.** Let now **Č** = **C*** with $\check{C}_{ij} = C^*_{ij}$. It will be the simplified form of the elasticity tensor that we are going to use in the remaining part of the paper. At the end, the coefficients will be replaced by their respective expression.

2.4. Action of R on *Č*

The action of ***R*** on ***Č*** gives:

$$\check{C} = R^t \check{C} R \quad (12)$$

let's write R in the reduced following form:

$$R = \begin{pmatrix} R_{2\theta} & 0_3 \\ 0_3 & r_\theta \end{pmatrix}$$

$$R^t = \begin{pmatrix} R^t_{2\theta} & 0_3 \\ 0_3 & r^t_\theta \end{pmatrix}$$

$$\check{C} = \begin{pmatrix} C_1 & C_2 \\ C_2^t & C_3 \end{pmatrix}$$

This reduced form helps us to simplify the calculation, and we get:

$$\check{C}' = \begin{pmatrix} R^t_{2\theta} C_1 R_{2\theta} & R^t_{2\theta} C_1 r_\theta \\ r^t_{2\theta} C_2^t R_{2\theta} & r^t_\theta C_3 r_\theta \end{pmatrix} \quad (13)$$

Let's denote $C_1' = R^t_{2\theta} C_1 R_{2\theta}$, $C_2' = r^t_{2\theta} C_2^t R_{2\theta}$, $C_2'^t = R^t_{2\theta} C_1 r_\theta$ and $C_3' = r^t_\theta C_3 r_\theta$. We can rewrite

$$\check{C}' = \begin{pmatrix} C_1' & C_2'^t \\ C_2' & C_3' \end{pmatrix} \quad (14)$$

We see that $\check{C}'$ is divided into three groups associated with C_1', C_2' and C_3' the transformation of each group is uncoupled from the others.

One can see that, the tensor ***C*** is divided into six groups by Ting [8]. By doing this, he found that the invariants of some groups contain components from different groups of $\boldsymbol{C_k}$, k = 1, 2, 3, ..., 6. Let's remark that, other authors (Lekhnttskii [18], Hearmon [19], Tsai [20]) have used the same decomposition as Ting but the transformations were written out explicitly, not in the matrix form.

3. References Results and Discussions: Invariants Determination

In the following subsections we are going to determine the invariants of each transformation separately. We have for each component of $\check{C}'$ six independent invariants.

3.1. The invariants of C_1'

The transformation of (13) gives us $C_1' = R_{2\theta}^t C_1 R_{2\theta}$, which can be seen as a miniature of the transformation of the 6x6 matrix $\check{C}'$. Then we evaluated the invariants of Č compared to their same quantity in *C*.

let's write:

$$C_1' = \begin{pmatrix} \check{C}_{11} & q_1 \\ q_1^t & a_1 \end{pmatrix} \quad (15)$$

$\check{C}_{11}$ is scalar, q_1 is vector and a_1, a 2x2 matrix.

The calculations give the following invariants:

- The coefficient (I_1)

$$\check{C}_{11}$$

- The length square (I_6)

$$q_1^2 = \check{C}_{12}^2 + \check{C}_{13}^2$$

- The trace of a_1 the reduced matrix issue to C_1' (I_2)

$$tr(a_1) = \check{C}_{22} + \check{C}_{33}$$

- The determinant of a_1 (I_{11})

$$\det(a_1) = \check{C}_{22}\check{C}_{33} - \check{C}_{23}^2$$

- The sum of two length squares L_1^2 issue to a_1 (I_{10})

$$L_1^2 = \check{C}_{22}^2 + \check{C}_{33}^2 + 2\check{C}_{23}^2$$

- The determinant of C_1' (I_{12})

$$\det\left(C_1'\right) = \check{C}_{11}\check{C}_{22}\check{C}_{33} + 2\check{C}_{12}\check{C}_{13}\check{C}_{23} - \check{C}_{11}\check{C}_{23}^2 - \check{C}_{22}\check{C}_{13}^2 - \check{C}_{33}\check{C}_{12}^2$$

3.2. The Invariants of C_3'

The transformation of (13) gives us $C_3' = r_\theta^t C_3 r_\theta$. In the same way, we evaluated the invariants of Č compared to their same quantity in ***C***.

let's write:

$$C_3' = \begin{pmatrix} a_3 & q_3 \\ q_3^t & \check{C}_{66} \end{pmatrix} \quad (16)$$

$\check{C}_{66}$ is scalar, q_3 is a vector and a_3 is a 2x2 matrix.

The calculations give the following invariants:

- The coefficient (I_3)

$$\check{C}_{66}$$

- The length square (I_7)

$$q_3^2 = \check{C}_{46}^2 + \check{C}_{56}^2$$

- The trace of a_3 the reduced matrix issue to C_3' (I_4)

$$tr(a_3) = \check{C}_{44} + \check{C}_{55}$$

- The determinant of a_3 (I_{14})

$$\det(a_3) = \check{C}_{44}\check{C}_{55} - \check{C}_{45}^2$$

- The sum of two length squares L_3^2 issue to a_3 (I_{13})

$$L_3^2 = \check{C}_{44}^2 + \check{C}_{55}^2 + 2\check{C}_{45}^2$$

- The determinant of C_3' (I_{15})

$$\det\left(C_3'\right) = \check{C}_{44}\check{C}_{55}\check{C}_{66} + 2\check{C}_{46}\check{C}_{56}\check{C}_{45} - \check{C}_{44}\check{C}_{56}^2 - \check{C}_{55}\check{C}_{46}^2 - \check{C}_{66}\check{C}_{45}^2$$

3.3. The Invariants of C_2'

Similarly, $C_2'^t = r_{2\theta}^t C_2^t R_{2\theta}$.

let's write:

$$C_2' = \begin{pmatrix} q_2^{(1)} & a_2 \\ \check{C}_{16} & q_2^{(2)} \end{pmatrix} \quad (17)$$

$\check{C}_{16}$ is a scalar, $q_3^{(i)}$ are vectors and a_2, a 2x2 matrix.

The calculation gives the following invariants:

- The coefficient (I_5)

$$\check{C}_{16}$$

- The length square (I_8)

$$\left(q_2^{(1)}\right)^2 = \check{C}_{14}^2 + \check{C}_{15}^2$$

- The length square (I_9)

$$\left(q_2^{(2)}\right)^2 = \check{C}_{26}^2 + \check{C}_{36}^2$$

- The determinant of a_2 (I_{17})

$$\det(a_2) = \check{C}_{24}\check{C}_{35} - \check{C}_{25}\check{C}_{34}$$

- The sum of two length squares L_2^2 issue to a_2 (I_{16})

$$L_3^2 = \check{C}_{24}^2 + \check{C}_{25}^2 + \check{C}_{34}^2 + \check{C}_{35}^2$$

- The determinant of C_2' (I_{18})

$$\det\left(C_2'\right) = \check{C}_{14}\left(\check{C}_{25}\check{C}_{36} - \check{C}_{26}\check{C}_{35}\right) + \check{C}_{15}\left(\check{C}_{26}\check{C}_{34} - \check{C}_{24}\check{C}_{36}\right) + \check{C}_{16}\left(\check{C}_{24}\check{C}_{35} - \check{C}_{25}\check{C}_{34}\right)$$

A total of eighteen invariants are found.

3.4. Summary of Invariants

Using relation (11), we replace the coefficients of $\check{C}_{ij}$ by their expressions, giving us the following invariants:

$$I_1 = \frac{1}{2}(C_{11} + 2C_{12} + C_{22})$$

$$I_2 = \frac{1}{2}(C_{11} - 2C_{12} + C_{22}) + C_{66}$$

$$I_3 = C_{33}$$

$$I_4 = C_{44} + C_{55}$$

$$I_5 = \frac{1}{\sqrt{2}}(C_{13} + C_{23})$$

$I_1 = 2\Phi_2$, $I_3 = \Phi_1$, $I_4 = \Phi_4$, $\sqrt{2}I_5 = \Phi_3$, where Φ_1 , Φ_3 , Φ_4 are the invariants of Ting.

$$I_6 = \frac{1}{4}(C_{11} - C_{22})^2 + \frac{1}{2}(C_{16} + C_{26})^2$$

$$I_7 = C_{34}^2 + C_{35}^2$$

$$I_8 = \frac{1}{2}\left[(C_{14} + C_{24})^2 + (C_{15} + C_{25})^2\right]$$

$I_7 = \psi_1$ and $2I_8 = \psi_6$, where ψ_1 and ψ_6 are once more Ting invariants.

$$I_9 = \frac{1}{2}(C_{13} - C_{23})^2 + C_{36}^2$$

$$I_{10} = \frac{1}{4}(C_{11} - 2C_{12} + C_{22})^2 + C_{66}^2 + (C_{16} - C_{26})^2$$

$$I_{11} = \frac{1}{2}\left[(C_{11} - 2C_{12} + C_{22})C_{66} - (C_{16} - C_{26})^2\right]$$

$$I_{12} = \left(C_{11}C_{22} - C_{12}{}^2\right)C_{66} + 4C_{12}C_{16}C_{26} - C_{11}C_{26}{}^2 - C_{22}C_{16}{}^2$$

$$I_{13} = C_{44}^2 + C_{55}^2 + 2C_{45}^2$$

$$I_{14} = C_{44}C_{55} - C_{45}^2$$

$I_{13} = \psi_3$ and $I_{14} = \psi_3'$, ψ_3 and ψ_3' being the invariants of Ting.

$$I_{15} = C_{33}C_{44}C_{55} + 2C_{34}C_{35}C_{45} - C_{44}C_{35}^2 - C_{55}C_{34}^2 - C_{33}C_{45}^2$$

$$I_{16} = \frac{1}{2}(C_{14} - C_{24})^2 + \frac{1}{2}(C_{15} - C_{25})^2 + C_{46}^2 + C_{56}^2$$

$$I_{17} = \frac{1}{\sqrt{2}}\left[C_{56}(C_{14} - C_{24}) - C_{46}(C_{15} - C_{25})\right]$$

$$\begin{aligned} I_{18} = {} & C_{36}(C_{15}C_{24} - C_{14}C_{25}) \\ & + C_{56}(C_{14}C_{23} - C_{13}C_{24}) \\ & + C_{46}(C_{13}C_{25} - C_{15}C_{23}) \end{aligned}$$

This is a proof that these eighteen invariants exist. Note that we can combine these invariants to get joins invariants.

In the following lines we will see their forms for isotropic materials like fiber composite materials that we can assimilate as isotropic.

4. Physical Signification: Isotropic Case

Materials are isotropic when in the elasticity tensor (Zuber [21] and Dieulesaint et al. [22]) $C_{11} = C_{22} = C_{33}$, $C_{12} = C_{13} = C_{23}$ and $C_{44} = C_{55} = C_{66}$. The remaining coefficients $C_{ij} = 0$.

We can see that $\frac{1}{2}(I_1 - I_4)$ and I_4 correspond to Lame coefficients respectively λ and μ. These two coefficients are sufficient to classify isotropic materials.

This proves that these eighteen invariants can be used for the classification of materials while waiting to make the 297 base useful.

5. Conclusion

In this work, we defined a rotation of SO(3) thanks to which we found eighteen independent invariants that we also called global invariants in a cartesian reference frame proving their existence. The invariants of the first order and some (quadratic) of the second degree have also been found by other authors such as Ahmad [5], Norris [6] and Ting [8]. Since these invariants (function of coefficients of $\check{C}$) are identical around the three axis for Cartesian base, it gives an advantage in the measurement of the elasticity tensor or in the mechanical characterization of materials.

About the question of knowing the type of materials that characterize each invariant, we treat the isotropic case which proves that these invariants can be useful for materials classification. It will be interested to give a mechanical interpretation and completed classification according to the invariants we have found.

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