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Numerical Determination of the Mean Value of an Elasticity Tensor by Integration over the Rotation Group with Haar Measure

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Abstract

Let **A** be a 3D symmetric elasticity tensor not necessary isotropic. If μ is an invariant measure on SO(3), then μ is a convex combinaison of the Haar measure. The nearest isotropic elasticity tensor is obtained by integrating the tensor **A** on the rotation group SO(3). For the numerical approach, we integrate the elasticity tensor on the unit ordinary ball B(0, 1).

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1 Introduction

In linear elasticity, the stress tensor and the strain tensor of a material are connected at a given temperature, by Hooke's law. Thus, each material is characterized by its elasticity tensor \mathbf{A} , but this correspondence is not unique. Indeed, given the explicit component of \mathbf{A} depends on the choice of an orthonormal basis in which are expressed tensor components. A change of orthonormal basis induces an action of the rotation group SO(3) on the space of elasticity tensors ($\mathbb{E}la$). Therefore, from the viewpoint of linear elasticity, describing all materials is to describe the orbits of the action of the rotation group SO(3) on $\mathbb{E}la$.

Chandwick et al. [1] proved that there are eight classes which can be put into correspondence with the eight classical symmetry groups as described by Forte and Vianello [2]: triclinic, monoclinic, tetragonal, trigonal, orthotropic, transversely isotropic, cubic and isotropic materials. We are interested here on the isotropic elasticity tensors.

Let A_0 be a raw elasticity tensor (because of the experimental errors) determined by any experimental method, e.g., the acoustical one presented by François et al. [3,4].

In the literature the least squares method is applied to research the nearest isotropic law. François et al. [4,5] propose an intrinsic function that creates from the raw tensor $\mathbf{A}_{\mathbf{0}}$ and the arbitrary base B a tensor $\mathbf{A}_{\mathbf{b}}$ which has the chosen symmetric group G. This function calculates the average of $\mathbf{A}_{\mathbf{0}}$ on its orbit according to G_B related to the base B. The natural symmetry base B_s is the one for which the relative discrepancy D(B) between $\mathbf{A}_{\mathbf{b}}$ and $\mathbf{A}_{\mathbf{0}}$ can be called the distance from $\mathbf{A}_{\mathbf{0}}$ to $\mathbf{A}_{\mathbf{s}}$; in other words the distance to the symmetric group G.

This approach was also developped by M. Vianello in [6] where he minimizes the distance between the raw elasticity tensor measured and its invariants polynomial decomposition.

There are also some methods of parameterization of SO(3) to determine the elasticity tensor. A. Boná et al.[7] propose a parametrization of the twenty-one-dimensional space of elasticity tensors by eighteen parameters and three Euler angles in such a way that Euler angles determine the orientation of a natural coordinate system. Six of these parameters represent the rigidity moduli of the elasticity tensor, an-other twelve parameters determine the six orthonormal eigentensors with respect to the three orthonormal eigenvectors.

Sandra Forte et al. [8] propose a decomposition based on the Haar integral. Using the property of the left and right invariance of the Haar integral, they calculate the restricted invariants on the space of elasticity tensors. The linear elasticity tensor is a linear combinaison of elements of the orbit centered at the origin.

The aim of this article is that we (effectively) calculated numerically the average on the group of SO(3) by performing (by the parameterization of Olinde Rodrigues) the integration on a threedimensional unit ball (discretized by finite elements).

The validation example is a numerical simulation (noisy isotropic law) and not an experimental measurement of the elastic coefficients of a real material.

All vector spaces, matrices, ect., considered in this paper are real.

Latin indices vary in the set $\{1, 2, 3\}$, save when they are used for indexing sequences, and sommation convention with respect to repeated indices is systematically used in conjunction with this rule.

Spaces of functions, vector fields, and symmetric matrix fields, defined over an open subset are respectively denoted by italic capitals, boldface Romain, and spacial Roman capitals.

2 Numerical Integration on SO(3)

2.1 Hooke's Law

Chandwick et al. [1]: in relation to some orthogonal basis, the components of the stress and strain tensors are σ_{ij} and ϵ_{ij} , respectively and Hooke's law takes the form $\sigma_{ij} = \mathbf{A}_{ijkl}\epsilon_{kl}$ where \mathbf{A}_{ijkl} are the components of the fourth-order elasticity tensor \mathbf{A} . The components of \mathbf{A} satisfy the symmetry relations $\mathbf{A}_{ijkl} = \mathbf{A}_{jikl} = \mathbf{A}_{ijlk} = \mathbf{A}_{klij}$, due to the symmetry of the stress and strain tensors and the requierement that no net work be done by an elastic material in a closed loading cycle.

2.2 Classical Determining of the Tensor A

Let **A** be an elasticity tensor. We are looking for the nearest isotropic elasticity tensor. Let us define the linar mapping : $\mathbf{H}(\epsilon) = \lambda \operatorname{tr}(\epsilon)\mathbf{I} + 2\mu\epsilon = \mathbf{A}\epsilon$. Hence, λ and μ are the unkown parameters since the 21 coefficients of **A** are given.

For the classical method, the problem leads to minimize $\mathcal{P}(\lambda, \mu) = \frac{1}{2} \text{tr} \left[(\mathbf{A} - \mathbf{H})^2 \right]$. \mathcal{P} is a second degree polynomial since \mathbf{H} and \mathbf{A} are explicited in Voigt normalized basis:

$$\mathbf{E_1} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}; \quad \mathbf{E_2} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}; \quad \mathbf{E_3} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}; \\ \mathbf{E_4} = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}; \quad \mathbf{E_5} = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}; \quad \mathbf{E_6} = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}$$

For the isotropic material, the elasticity tensor is written in Voigt basis:

$$\mathbf{A} = \begin{pmatrix} \lambda + 2\mu & \lambda & \lambda & 0 & 0 & 0 \\ \lambda & \lambda + 2\mu & \lambda & 0 & 0 & \\ \lambda & \lambda & \lambda + 2\mu & 0 & 0 & 0 \\ 0 & 0 & 0 & \mu & 0 & 0 \\ 0 & 0 & 0 & \mu & 0 & \\ 0 & 0 & 0 & 0 & 0 & \mu \end{pmatrix}$$

One can explicit \mathbf{H} and \mathbf{A} on the basis constituted of five deviatorics and a spherical matrices:

$$\mathbf{H} = \begin{pmatrix} 2\mu & (0) & & \\ (0) & \ddots & & 0 \\ & & 2\mu & \\ & 0^T & & 3\lambda + 2\mu \end{pmatrix} \quad \text{and } \mathbf{A} = \begin{pmatrix} \mathbf{S} & \mathbf{v} \\ \mathbf{v}^T & \alpha \end{pmatrix}$$

where **S** is a 5×5 symmetric matrix, $\mathbf{v} \in \mathbb{R}^5$ and $\alpha \in \mathbb{R}$.

Let \mathbf{I}_5 be the 5 × 5 identity matrix, then the polynomial $\mathcal{P}(\lambda, \mu)$ is written

$$\mathcal{P}(\lambda,\mu) = \frac{1}{2} \left[\alpha - (3\lambda + 2\mu) \right]^2 + 10\mu^2 - 2\mu \mathrm{tr} \left[\left(\mathbf{S} - 2\mu \mathbf{I}_5 \right)^2 \right] + \mathbf{v}^T \mathbf{v}.$$

For the classical approach, one has:

$$3\lambda + 2\mu = \alpha$$
 and $2\mu = \frac{1}{5} \text{tr} \mathbf{S}.$

This choice is justified by the fact that the elasticity tensor is diagonal in this basis and calculations are more simple.

Let us develop a new approach inspired from Sourriau [9].

2.3 Integration on the Rotation Group SO(3)

SO(3) is a semisimple Lie group or unimodular group.

Let **R** be the 3×3 rotation matrix. We define the Haar positive left invariant measure $d\mu$. Since SO(3) is unimodular group, this measure is also right invariant (see [10]).

First, we will parametrize rotation matrices with Rodrigues coefficients.

2.4 Rotation Parameterization

Consider a rotation with the angle θ around the unit vector **u**, the Gibbs formula is given by:

$$\mathbf{R} = \cos(\theta)\mathbf{I}_3 + \sin(\theta)j(\mathbf{u}) + (1 - \cos(\theta))\mathbf{u} \otimes \mathbf{u}, \ \theta \in [0, \pi],$$

where we define the matrix $j(\mathbf{u}) = \begin{pmatrix} 0 & -u_3 & u_2 \\ u_3 & 0 & -u_1 \\ -u_2 & u_1 & 0 \end{pmatrix}$.

The Rodrigues coefficients are:

$$m_0 = \cos\left(\frac{\theta}{2}\right); \quad m_i = \sin\left(\frac{\theta}{2}\right)u_i, \ i = 1, 2, 3.$$

If we denote $\mathbf{m} = (m_1, m_2, m_3)^T$, we can rewrite the Gibbs formula:

$$\mathbf{R} = \left(2m_0^2 - 1\right)\mathbf{I}_3 + 2m_0j(\mathbf{m}) + 2\mathbf{m}\otimes\mathbf{m}.$$

This expression is second degree respect to the parameters.

Since $0 \le \theta \le \pi$, the real $m_0 \in [0, 1]$. From $m_0 \ge 0$ and $(m_0)^2 + (m_1)^2 + (m_2)^2 + (m_3)^2 = 1$, one has: $m_0 = \sqrt{1 - \mathbf{m} \cdot \mathbf{m}}$. Therefore the vector \mathbf{m} is an element of the unit compact ball B(0, 1), and consequently SO(3) is compact and we can parametrize SO(3) by the Rodrigues parameters m_1 , m_2 and m_3 [11,12].

Proposition 2.1. The unique Haar measure is

$$d\mu = \frac{1}{\pi^2} \frac{dm_1 dm_2 dm_3}{m_0}.$$
 (2.1)

Comments Instead of integrating on SO(3) one integrates on the unit ordinary ball B(0,1):

$$\int_{SO(3)} f(\mathbf{R}) d\mu = \int_{B(0,1)} f(\mathbf{R}(\mathbf{m})) \frac{1}{\pi^2} \frac{dm_1 dm_2 dm_3}{\sqrt{1 - \mathbf{m} \cdot \mathbf{m}}}$$

Let us verify that $\int_{B(0,1)} \frac{dm_1 dm_2 dm_3}{m_0} = \pi^2$.

$$\int_{B(0,1)} \frac{dm_1 dm_2 dm_3}{\sqrt{1-\mathbf{m}.\mathbf{m}}} = \int_0^1 \frac{S(r)}{\sqrt{1-r^2}} dr \ S(r) \text{ is the sphere surface}$$
$$= 4\pi \int_0^1 \frac{r^2 dr}{\sqrt{1-r^2}} = \pi \int_0^\pi (1-\cos\theta) \, d\theta = \pi^2.$$

Proof. of the proposition : We seek the Haar measure in density measure form

$$d\mu = \rho(\mathbf{m}) dm_1 dm_2 dm_3.$$

Let us prove that the left-invariance imposes that

$$\rho(\mathbf{m}) = \frac{C}{\sqrt{1 - (m_1)^2 - (m_2)^2 - (m_3)^2}}$$

where C is a constant.

One can verify that the right-invariance leads to the same conclusion.

The definition $\mathbf{R}' = \Omega \mathbf{R}, \ \Omega \in SO(3)$ leads to [12]

$$egin{cases} n_0' &= m_0 n_0 - \mathbf{m}. \mathbf{n} \ \mathbf{m}' &= m_0 \mathbf{n} + \mathbf{m} \wedge \mathbf{n}. \end{cases}$$

The invarianbility of the Haar measure $d\mu = \rho(\mathbf{m})d\mathbf{m}$ is equivalent to the condition

$$\rho(\mathbf{m}')\mathbf{dm}' = \rho(\mathbf{m})\mathbf{dm}.$$
(2.2)

Let the matrix **J** be the jacobean of the mapping which transforms **m** to **m**'. Haar measure imposes that for all **n**, $\rho(\mathbf{m}')\det \mathbf{J} = \rho(\mathbf{m})$.

Now, let us calculate the jacobean **J**. First, we verify that $(m'_0)^2 + \mathbf{m}' \cdot \mathbf{m} = 1$. Indeed,

$$\begin{pmatrix} m'_{0} \\ \mathbf{m}' \end{pmatrix} = \begin{pmatrix} n_{0} & -\mathbf{n}^{T} \\ \mathbf{n} & n_{0}\mathbf{I}_{3} - j(\mathbf{n}) \end{pmatrix} \begin{pmatrix} m_{0} \\ \mathbf{m} \end{pmatrix} \text{ where } j(\mathbf{n}) = \begin{pmatrix} 0 & -n_{3} & n_{2} \\ n_{3} & 0 & -n_{1} \\ -n_{2} & n_{1} & 0 \end{pmatrix}$$
$$= n_{0}\mathbf{I}_{4} + n_{1} \begin{pmatrix} 0 & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & -1 & 0 \end{pmatrix} + n_{2} \begin{pmatrix} 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix} + n_{3} \begin{pmatrix} 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \\ 0 & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}$$

The product

$$\begin{pmatrix} n_0 & -\mathbf{n}^T \\ -\mathbf{n} & n_0\mathbf{I}_3 + j(\mathbf{n}) \end{pmatrix} \begin{pmatrix} n_0 & -\mathbf{n}^T \\ \mathbf{n} & n_0\mathbf{I}_3 - j(\mathbf{n}) \end{pmatrix}$$

is the 4×4 identity matrix.

Secondly, to calculate the jacobean one can write

$$\begin{pmatrix} \delta m_0' \\ \delta \mathbf{m}' \end{pmatrix} = \begin{pmatrix} n_0 & -\mathbf{n}^T \\ \mathbf{n} & n_0 \mathbf{I}_3 - j(\mathbf{n}) \end{pmatrix} \begin{pmatrix} \delta m_0' \\ \delta \mathbf{m}' \end{pmatrix}$$

Since one has $\delta m_0 = -\frac{1}{m_0} \mathbf{m} \cdot \delta \mathbf{m}$ and $\delta m_0 = \frac{1}{m'_0} \mathbf{m'} \cdot \delta \mathbf{m'}$, therefore

$$\begin{pmatrix} \delta m_0' \\ \delta \mathbf{m}' \end{pmatrix} = \begin{pmatrix} -\frac{\mathbf{m}^T}{m_0} \\ \mathbf{I}_3 \end{pmatrix} \delta \mathbf{m}$$

Finaly, the jacobean matrix is the 3×3 matrix

$$\mathbf{J} = \begin{pmatrix} 0 & \mathbf{I}_3 \\ 0 & \mathbf{I}_3 \\ 0 & \end{pmatrix} \begin{pmatrix} n_0 & -\mathbf{n}^T \\ \mathbf{n} & n_0 \mathbf{I}_3 - j(\mathbf{n}) \end{pmatrix} \begin{pmatrix} -\frac{\mathbf{m}^T}{m_0} \\ \mathbf{I}_3 \end{pmatrix}.$$

Once we calculate **J**, one realizes, due to the compatibility conditions, that the condition (2.2) is only possible if $\rho(\mathbf{m}) = \frac{\text{constant}}{m_0}$.

2.5 Rotation Group Action on the Elasticity Tensor

Let $\mathbb{E}la$ be a 3D strain space. This space is Euclidean space if we consider the scalar product:

$$E \times E \longrightarrow \mathbb{R}$$
$$(\epsilon, \epsilon') \longmapsto \operatorname{tr}(\epsilon \epsilon')$$

An elasticity tensor is a self-adjoint linear mapping.

We define a SO(3) group action on the six-dimensional vectorial space of elasticity tensors by:

$$\forall \epsilon \in E, \forall \mathbf{R} \in SO(3) : \mathbf{A}_R(\epsilon) = \mathbf{R}\mathbf{A}(\mathbf{R}^{-1}\epsilon\mathbf{R})\mathbf{R}^{-1}$$

We denote by $\mathbf{R}(\mathbf{A}) = \mathbf{A}_R$ this action. For two rotations \mathbf{R}_1 and \mathbf{R}_2 we can verify that

$$(\mathbf{R}_1\mathbf{R}_2)(\mathbf{A})(\epsilon) = \mathbf{R}_1\mathbf{R}_2\mathbf{A}\left(\mathbf{R}_2^{-1}\mathbf{R}_1^{-1}\epsilon\mathbf{R}_1\mathbf{R}_2\right)\mathbf{R}_2^{-1}\mathbf{R}_1^{-1} = \mathbf{R}_1\left(\mathbf{R}_2\left(\mathbf{A}\right)\right)(\epsilon).$$

Then, for the elasticity tensors, the action satisfies the group action law

$$(\mathbf{R}_1\mathbf{R}_2)(\mathbf{A}) = \mathbf{R}_1(\mathbf{R}_2(\mathbf{A}))$$

if **A** is isotropic, therefore $\mathbf{R}(\mathbf{A}) = \mathbf{A}$ for all **R**. If due to steps approximation, the tensor **A** is not isotropic, one can take the combination of **R** on the SO(3) group

$$\mathbf{H} = \int_{SO(3)} \mathbf{R}(\mathbf{A}) d\mu.$$

Proposition 2.2. This combination of \mathbf{R} on the SO(3) group is isotropic.

Remark 2.1. For the numerical implementation, we use the Rodrigues coefficients to integrate:

$$\mathbf{H} = \frac{1}{\pi^2} \int_{B(0,1)} \mathbf{R}(\mathbf{m}) \mathbf{A} \frac{d\mathbf{m}}{m_0}.$$
 (2.3)

We calculate \mathbf{H} by the finite element method.

Proposition 2.3. $\int_{SO(3)} \mathbf{R}(\mathbf{A}) d\mu$ is the solution of the minimization problem of the classical method.

Proof. this proposition is due from the fact that SO(3) preserves the lengths. Let us prove that

$$3\mu' + 2\lambda' = \alpha$$
 and $2\mu' = \frac{1}{5} \text{tr}\mathbf{S}$

For the first assertion, one has $\mathbf{R}(\mathbf{A}) = \mathbf{R}\mathbf{A} \left(\mathbf{R}^{-1} \epsilon \mathbf{R}\right) \mathbf{R}^{-1}$. Let $\epsilon = \mathbf{I}_3$, we obtain $\mathbf{R}(\mathbf{A}) = \mathbf{R}\mathbf{A}(\mathbf{I}_3)\mathbf{R}^{-1}$.

We can rewrite $\mathbf{A} = \alpha \frac{\mathbf{I}_3}{\sqrt{3}} \otimes \frac{\mathbf{I}_3}{\sqrt{3}}$; therefore $\mathbf{A}\mathbf{I}_3 = \alpha \frac{\mathbf{I}_3}{3}$ and tr $[\mathbf{I}_3 (\mathbf{R}(\mathbf{A})\mathbf{I}_3)] = \text{tr} [\mathbf{I}_3\mathbf{A}(\mathbf{I}_3)] = \alpha$.

Furthermore, from the formula $\mathbf{H}(\mathbf{A}) = \frac{1}{\pi^2} \int_{B(0,1)} \mathbf{R}(\mathbf{m}) \mathbf{A} \frac{d\mathbf{m}}{m_0}$, we conclude

tr
$$[\mathbf{I}_3\mathbf{H}(\mathbf{I}_3)] = 3\lambda' + 2\mu' = \frac{1}{\pi^2}\alpha \int_{B(0,1)} \frac{d\mathbf{m}}{m_0} = \alpha.$$

For the second one, we rewrite

$$\mathbf{H}(\mathbf{A}) - \alpha \frac{\mathbf{I}_3}{\sqrt{3}} \otimes \frac{\mathbf{I}_3}{\sqrt{3}} = \frac{1}{\pi^2} \int_{B(0,1)} \mathbf{R}(\mathbf{m}) \left[\mathbf{A} - \alpha \frac{\mathbf{I}_3}{\sqrt{3}} \otimes \frac{\mathbf{I}_3}{\sqrt{3}} \right] \frac{d\mathbf{m}}{m_0}$$

Let us use this lemma:

Lemma 2.1. The group action conserves the trace.

So, if we take the trace of both members, we get

$$10\mu' = \frac{1}{\pi^2} \operatorname{tr} \mathbf{S} \int_{B(0,1)} \frac{d\mathbf{m}}{m_0} = \operatorname{tr} \mathbf{S}.$$

Proof. of the lemma : we must prove that $\mathbf{R}(\mathbf{A})$ and \mathbf{A} have the same trace.

One can take $\mathbf{R}(\mathbf{A}) = e^{-\theta \mathbf{M}} \mathbf{A} e^{\theta \mathbf{M}}$ with $\mathbf{M} \epsilon = \epsilon j(\alpha) - j(\alpha) \epsilon$. Then,

$$\operatorname{tr} \mathbf{H} = \int_{SO(3)} \operatorname{tr}(\mathbf{A}) d\mu = \operatorname{tr} \mathbf{A} \int_{SO(3)} d\mu = \operatorname{tr} \mathbf{A}.$$

3 Numerical Example

Instead of analytically integrating Eq. 2.3, a numerical approach is applied. The unit ordinary ball B(0,1) is discretized into 270424 tetrahedral elements, as shown in Figure (1). Initial values



Figure 1: Discretized ball with 270424 elements

of material constants are chosen as: $\lambda = 50$ MPa, $\mu = 10$ MPa. A perturbation is applied to the elasticity tensor **A** by

$$A_{ijkl} = A_{ijkl}^0 + 0.01[1 + (i-1)(j-1) - 0.32(k-1)(l-1)]$$
(3.1)

For numerical purpose, it is more convenient to write the elasticity tensor in a symmetric matrix form based on Voigt's representation:

	70.01	50.0068	49.9972	0.01	0.0036	0.01]
$\left[\mathbf{A} ight]_{o} =$		70.0168	50.0072	0.02	0.0136	0.02	
			70.0372	0.05	0.0436	0.05	(2.9)
				10.01	0.0036	0.01	(3.2)
					10.0236	0.0036	
	L					10.01	

After integration, we obtain new material constants as: $\lambda = 46.9757$ MPa, $\mu = 9.4004$ MPa. The elasticity matrix becomes:

$\left[\mathbf{A} ight]_n =$	65.7766	46.9757 65.7765	46.9758 46.9757 65.7762	$\begin{array}{c} -0.000482 \\ -0.000264 \\ -0.000223 \\ 9.40039 \end{array}$	$\begin{array}{c} -0.000257\\ -0.000381\\ -0.000085\\ -0.000364\\ 9.40026\end{array}$	$\begin{array}{c} -0.000589\\ -0.000297\\ -0.000118\\ -0.000146\\ -0.000306\\ 9.40038 \end{array}$	(3.3)
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We remark that the two coefficients of Lamé are determined with good accuracy: the first coefficient λ is determined with 6% accuracy, and the second μ is determined with 3% accuracy.

4 Conclusion

Based on the Souriau variational approach, we established that the nearest isotropic elasticity tensor of a measured elasticity tensor can be determined by integration on the rotation group SO(3). The rotation matrices parametrization within Rodrigues coefficients leads to integrate on the unit ordinary ball B(0,1). The unit ball is discretized by the finite element approach. The numerical results confirm the approach developped. The accuracies obtained on the Lamé's coefficients are very good.

In this work, the elasticity tensor was identified. We propose in the future to extend this approach to other symmetry group and this work is being undertaken.

Competing Interests

The authors declare that no competing interests exist.

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