Bornes supérieures à la distance à l'élasticité cubique ou orthotrope

R. Desmorat, B. Kolev

Laboratoire de Mécanique Paris-Saclay (LMPS)

GDR GDM – La Rochelle – 26 juin 2024

OUTLINE

COMPORTEMENT D'UN RESSORT/BARRE ÉLASTIQUE

Ressort de raideur k:

$$F = k\,\Delta\ell = k\,(\ell - \ell_0)$$

Barre de section S_0, de longueur initiale ℓ_0, de raideur E:

$$\sigma = \frac{F}{S_0} = E\,\frac{\Delta\ell}{\ell_0} = E\epsilon, \qquad E = \frac{k\ell_0}{S_0}$$

Contrainte σ et (petite) déformation ϵ

$$\sigma := \frac{F}{S_0}, \qquad \epsilon := \frac{\Delta\ell}{\ell_0}$$

LOI D'ÉLASTICITÉ TRIDIMENSIONNELLE

Les lois de comportement 3D font intervenir les tenseurs

- (variable) des contraintes $\boldsymbol{\sigma} = (\sigma^{ij})$, contravariant d'ordre 2,
- (variable) des petites déformations $\boldsymbol{\epsilon} = (\epsilon_{ij})$, covariant d'ordre 2,
- (constitutif) d'élasticité $\mathbf{E} = (E^{ijkl})$, contravariant d'ordre 4,

Elasticité linéaire 3D

La relation scalaire $\sigma = E\epsilon$ se généralise,

$$\boldsymbol{\sigma} = \mathbf{E} : \boldsymbol{\epsilon}, \qquad \sigma^{ij} = E^{ijkl}\epsilon_{kl}, \qquad E^{ijkl} = E^{jikl} = E^{klij}.$$

Déplacement $\boldsymbol{u}$,

$$\boldsymbol{\epsilon} = \frac{1}{2}\left(\nabla \boldsymbol{u}^\flat + (\nabla \boldsymbol{u}^\flat)^t\right), \qquad \epsilon_{ij} = \frac{1}{2}\left(u_{i,j} + u_{j,i}\right).$$

LOI D'ÉLASTICITÉ TRIDIMENSIONNELLE

Les lois de comportement 3D font intervenir les tenseurs,

- des contraintes $\boldsymbol{\sigma} = (\sigma^{ij})$, contravariant d'ordre 2,
- des (petites) déformations $\boldsymbol{\epsilon} = (\epsilon_{ij})$, covariant d'ordre 2,
- d'élasticité $\mathbf{E} = (E^{ijkl})$, contravariant d'ordre 4,

Elasticité linéaire, en base orthonormée,

La relation scalaire $\sigma = E\epsilon$ se généralise,

$$\boldsymbol{\sigma} = \mathbf{E} : \boldsymbol{\epsilon}, \qquad \sigma_{ij} = E_{ijkl}\epsilon_{kl}, \qquad E_{ijkl} = E_{jikl} = E_{klij}.$$

Déplacement $\boldsymbol{u}$,

$$\boldsymbol{\epsilon} = \frac{1}{2}\left(\nabla \boldsymbol{u}^\flat + (\nabla \boldsymbol{u}^\flat)^t\right), \qquad \epsilon_{ij} = \frac{1}{2}\left(u_{i,j} + u_{j,i}\right).$$

Elasticité linéaire isotrope

$$\boldsymbol{\sigma} = 2\mu\,\boldsymbol{\epsilon} + \lambda\,\mathrm{tr}\,\boldsymbol{\epsilon}\,\mathbf{1} = 2G\,\boldsymbol{\epsilon}^D + K\;\mathrm{tr}\,\boldsymbol{\epsilon}\,\mathbf{1},$$

$$\left(\sigma_{ij} = 2\mu\epsilon_{ij}^D + \lambda\epsilon_{kk}\,\delta_{ij} = 2G\,\epsilon_{ij}^D + K\epsilon_{kk}\,\delta_{ij}\right),$$

$$G = \mu = \frac{E}{2(1+\nu)}, \qquad K = \frac{1}{3}(2\mu + 3\lambda) = \frac{E}{3(1-2\nu)}.$$

Tenseur d'élasticité isotrope

$$\mathbf{E} = 2\mu\,\mathbf{I} + \lambda\,\mathbf{1}\otimes\mathbf{1}, \qquad \left(E_{ijkl} = \mu\,(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}) + \lambda\,\delta_{ij}\delta_{kl}\right)$$

$$= 2G\,\mathbf{J} + K\,\mathbf{1}\otimes\mathbf{1}, \qquad \left(E_{ijkl} = 2G\,(I_{ijkl} - \frac{1}{3}\delta_{ij}\delta_{kl}) + K\,\delta_{ij}\delta_{kl}\right).$$

Elasticité linéaire isotrope

$$\boldsymbol{\sigma} = 2\mu\,\boldsymbol{\epsilon} + \lambda\,\mathrm{tr}\,\boldsymbol{\epsilon}\,\mathbf{1} = 2G\,\boldsymbol{\epsilon}^D + K\;\mathrm{tr}\,\boldsymbol{\epsilon}\,\mathbf{1},$$

$$\left(\sigma_{ij} = 2\mu\epsilon_{ij}^D + \lambda\epsilon_{kk}\,\delta_{ij} = 2G\,\epsilon_{ij}^D + K\epsilon_{kk}\,\delta_{ij}\right),$$

$$G = \mu = \frac{E}{2(1+\nu)}, \qquad K = \frac{1}{3}(2\mu + 3\lambda) = \frac{E}{3(1-2\nu)}.$$

Tenseur d'élasticité isotrope

$$\mathbf{E} = 2\mu\,\mathbf{I} + \lambda\,\mathbf{1}\otimes\mathbf{1}, \qquad \left(E_{ijkl} = \mu\,(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}) + \lambda\,\delta_{ij}\delta_{kl}\right)$$

$$= 2G\,\mathbf{J} + K\,\mathbf{1}\otimes\mathbf{1}, \qquad \left(E_{ijkl} = 2G\,(I_{ijkl} - \frac{1}{3}\delta_{ij}\delta_{kl}) + K\,\delta_{ij}\delta_{kl}\right).$$

Tenseur de souplesse isotrope

$$\mathbf{S} = \mathbf{E}^{-1} = \frac{1+\nu}{E}\,\mathbf{I} - \frac{\nu}{E}\,\mathbf{1}\otimes\mathbf{1}, \qquad \left(S_{ijkl} = \frac{1+\nu}{E}\,I_{ijkl} - \frac{\nu}{E}\,\delta_{ij}\delta_{kl}\right)$$

$$= \frac{1}{2G}\,\mathbf{J} + \frac{1}{9K}\,\mathbf{1}\otimes\mathbf{1}, \qquad \left(S_{ijkl} = \frac{1}{2G}\,J_{ijkl} + \frac{1}{9K}\,\delta_{ij}\delta_{kl}\right).$$

POLYCRISTAUX (EX: MÉTAUX)

Un matériau polycristallin est un matériau solide constitué d'une multitude de petits (mono)cristaux de taille et d'orientation variées.
Son comportement macroscopique peut être isotrope.

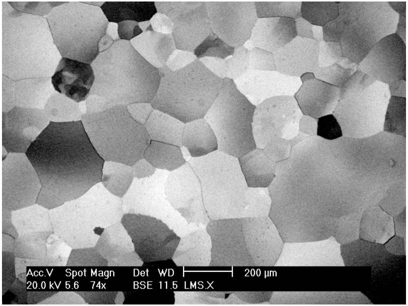


Figure: Observation MEB en imagerie d'électrons rétrodiffusés d'un polycristal de zirconium après polissage mécanique et électrolytique (d'après D. Cadelmaison).

POLYCRISTAUX ORTHOTROPES

Un matériau polycristallin est un matériau solide constitué d'une multitude de petits (mono)cristaux de taille et d'orientation variées.
Après laminage, son comportement macroscopique peut être orthotrope.

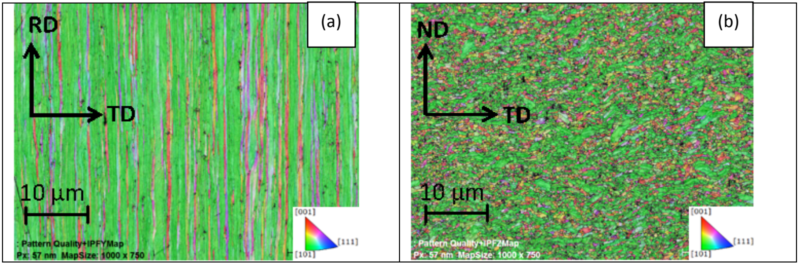


Figure: Acier "14%Cr 14 ferritic ODS" (Oxide Dispersion Strengthened, Fe-14Cr-1W-0.3Ti-0.25Y_2O_3, observation EBSD, Jaumier et al, 2019):
(a) longitudinal section, (b) transverse section.

MONOCRISTAUX CUBIQUES D'AUBES DE MOTEURS D'HÉLICOPTÈRES

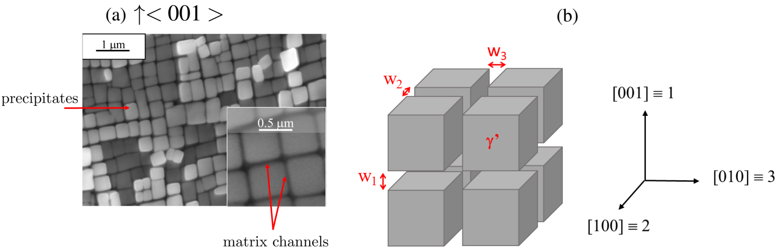


Figure 1.2 – Example of the initial cubic microstructure of Single Crystal Superalloys: (a) SEM observation of a crystal oriented along $< 001 >$ (Cormier (2006), MC2 alloy) and (b) schematic representation of the microstructure.

BASE NATURELLE D'ANISOTROPIE

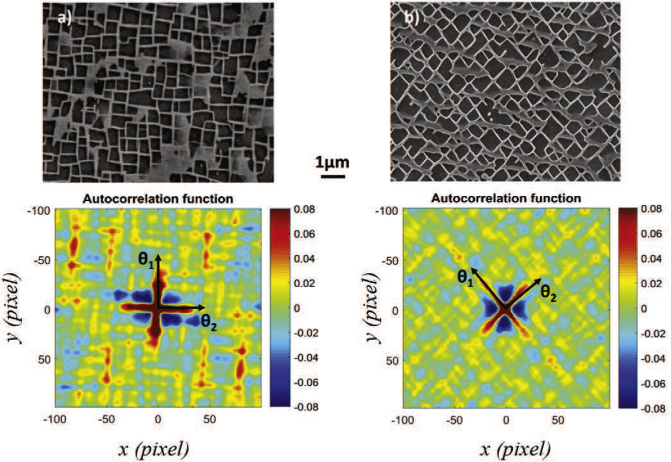


Figure: a) CMSX4 ⟨001⟩ γ/γ' cuboidal microstructure and autocorrelation function; b) ⟨111⟩ cuboidal microstructure and autocorrelation function (Caccuri et al, 2018).

Normal form

An elasticity tensor $\mathbf{E}$ in the symmetry stratum $\Sigma_{[G]}$ (of symmetry class $[G]$) may have exactly as symmetry group the canonical representative group G,

$$g \star \mathbf{E} = \mathbf{E}, \quad \forall g \in G,$$

where $(g \star \mathbf{E})_{ijkl} = g_{ip} g_{jq} g_{kr} g_{ls} E_{pqrs}$.

In that case, we say that $\mathbf{E}$ is in its normal form (expressed in its natural basis).

Example (of cubic symmetry, in natural cubic basis)

When $G = \mathbb{O}$, elasticity tensors in cubic normal form are written as

$$[\mathbf{E}] = \begin{pmatrix} E_{1111} & E_{1122} & E_{1122} & 0 & 0 & 0 \\ E_{1122} & E_{1111} & E_{1122} & 0 & 0 & 0 \\ E_{1122} & E_{1122} & E_{1111} & 0 & 0 & 0 \\ 0 & 0 & 0 & 2E_{1212} & 0 & 0 \\ 0 & 0 & 0 & 0 & 2E_{1212} & 0 \\ 0 & 0 & 0 & 0 & 0 & 2E_{1212} \end{pmatrix},$$

in Kelvin matrix representation.

Problématique mécanique

Les lois de comportement[1] sont formulées pour des symétries matérielles initiales particulières

- isotropie $[\mathrm{O}(3)]$,
- symétrie cubique $[\mathbb{O}]$, orthotropie $[\mathbb{D}_2]$.

Des essais mécaniques permettent de mesurer les paramètres matériaux bruités (ici les E_{ijkl}, Arts, 1993, François, 1995).

Questions

- Quelle est la base naturelle d'anisotropie ? Réponse mécanique préférée.
- Quelles sont les paramètres d'élasticité du tenseur $\mathbf{E}$ le plus proche d'une classe de symétrie $[G]$ donnée ?
- A quelle distance $d(\mathbf{E}, [G])$ le tenseur $\mathbf{E}$ est il de la strate de symétrie $\Sigma_{[G]}$ correspondante ?
- Solution approchées ? (bornes supérieures $M(\mathbf{E}, [G]) \geq d(\mathbf{E}, [G])$)

[1] élasto-(visco-)plastiques couplées ou non à l'endommagement.

Outline

Distance to a symmetry class $[G]$

Even if some analytical attempts exist (Vianello, 1997, Stahn et al, 2020), the distance to an elasticity symmetry class problem (Gazis et al, 1963) is often

- solved numerically, following Arts et al (1991, 1993) and François et al (1995, 1996, 1998),
- using the parameterization by a rotation g:

$$d(\mathbf{E}_0, [G]) := \min_{\mathbf{E} \in \overline{\Sigma}_{[G]}} \|\mathbf{E}_0 - \mathbf{E}\| = \min_{g \in \mathrm{SO}(3)} \|\mathbf{E}_0 - g \star \mathbf{R}_G(g^t \star \mathbf{E}_0)\|$$

- G is a symmetry group ($\mathbb{Z}_2$, $\mathbb{D}_2$, $\mathbb{D}_3$, $\mathbb{D}_4$, $\mathbb{O}$, $\mathrm{O}(2)$, $\mathrm{SO}(3)$, Forte–Vianello, 1996),
- $\mathbf{R}_G(\mathbf{E}) = \frac{1}{|G|} \sum_{g \in G} g \star \mathbf{E}$ is the Reynolds (group averaging) operator,
- $\mathbf{E} = g_{opt} \star \mathbf{R}_G(g_{opt}^t \star \mathbf{E}_0)$.

Distance to a symmetry class $[G]$

Even if some analytical attempts exist (Vianello, 1997, Stahn et al, 2020), the distance to an elasticity symmetry class problem (Gazis et al, 1963) is often

- solved numerically, following Arts et al (1991, 1993) and François et al (1995, 1996, 1998),
- using the parameterization rotation g / normal form $\mathbf{A}$ (Dellinger, 2005):

$$d(\mathbf{E}_0, [G]) := \min_{\mathbf{E}\in\overline{\Sigma}_{[G]}} \|\mathbf{E}_0 - \mathbf{E}\| = \min_{g,\mathbf{A}} \|\mathbf{E}_0 - g \star \mathbf{A}\|$$

- G is a symmetry group ($\mathbb{Z}_2$, $\mathbb{D}_2$, $\mathbb{D}_3$, $\mathbb{D}_4$, $\mathbb{O}$, $\mathrm{O}(2)$, $\mathrm{SO}(3)$, Forte–Vianello, 1996),
- $\mathbf{R}_G(\mathbf{A}) = \frac{1}{|G|}\sum_{g\in G} g \star \mathbf{A}$ is the Reynolds (group averaging) operator,
- $\mathbf{E} = g_{opt} \star \mathbf{A}_{opt}$.

OUTLINE

Upper bounds estimates rather than distances

For 3D elasticity, upper bounds estimates of the distance to a symmetry stratum have been formulated

- by Gazis, Tadjbakhsh and Toupin (1963) for cubic symmetry,
- by Klimeš (2018) for transverse isotropy,
- and by Stahn, Müller and Bertram (2020) for all symmetry classes, using a second-order tensor $\mathbf{t}$ (a covariant) of the elasticity tensor introduced by Backus (1970). This covariant is assumed to carry the likely symmetry coordinate system of $\mathbf{E}_0$.
- by us (2024), a second order tensor $\mathbf{a}$ (not a covariant) being assumed to carry the likely symmetry coordinate system.

All second-order covariants of an exactly cubic elasticity tensor are isotropic. Therefore, for a material expected to be cubic, a methodology based on second-order covariants is probably meaningless.

INVARIANTS /COVARIANTS OF THE ELASTICITY TENSOR

Covariants of a tensor **E** satisfy the rule, $\forall g \in \mathrm{SO}(3)$,

$$\mathbf{C}(g \star \mathbf{E}) = g \star \mathbf{C}(\mathbf{E}), \qquad \Big(I(g \star \mathbf{E}) = I(\mathbf{E}) \text{ for invariants } I(\mathbf{E}) \Big).$$

A covariant $\mathbf{C}(\mathbf{E})$ of **E** inherits the symmetry of **E**:
$\mathbf{C}(\mathbf{E})$ has at least the symmetry of **E**, $G_{\mathbf{E}} \subset G_{\mathbf{C}(\mathbf{E})}$.

Ex: harmonic decomposition of **E** (Backus, 1970, Cowin, 1989, Baerheim, 1993):

$$\mathbf{E} = (\lambda, \mu, \mathbf{d}', \mathbf{v}', \mathbf{H}) \in \mathbb{H}^0 \oplus \mathbb{H}^0 \oplus \mathbb{H}^2 \oplus \mathbb{H}^2 \oplus \mathbb{H}^4$$

- The quantities

$$\lambda = \lambda(\mathbf{E}), \quad \mu = \mu(\mathbf{E}), \quad \mathbf{d}' = \mathbf{d}'(\mathbf{E}), \quad \mathbf{v}' = \mathbf{v}'(\mathbf{E}), \quad \mathbf{H} = \mathbf{H}(\mathbf{E}),$$

  are covariants $\mathbf{C}(\mathbf{E})$ of **E** (of degree one and resp. order 0, 0, 2, 2 and 4).
- λ, μ / $\mathbf{d}'(\mathbf{E}), \mathbf{v}'(\mathbf{E}), \mathbf{H}(\mathbf{E})$ are linear invariants / covariants of **E**.

POLYNOMIAL COVARIANTS

- There exist polynomial covariants of higher degree, for example (Boehler et al, 1994)

$$\mathbf{d}_2(\mathbf{H}) := \mathbf{H} \,\vdots\, \mathbf{H}, \qquad (i.e.,\ (\mathbf{d}_2)_{ij} = H_{ipqr}H_{pqrj}),$$

- The algebra of (totally symmetric) polynomial covariants of the elasticity tensor has been defined by Olive et al (2021).
- A minimal integrity basis for the invariant algebra of $\mathbf{H} \in \mathbb{H}^4$ has been derived in (Boehler et al, 2021) (it is of cardinal 9).
- A minimal integrity basis for the invariant algebra of $\mathbf{E}$ has been derived in (Auffray et al, 2021) and (Olive et al, 2021) (it is of cardinal 294).
- A minimal integrity basis for the covariant algebra of $\mathbf{H} \in \mathbb{H}^4$ has been derived in (Olive et al, 2021) (it is of cardinal 70).

LITERATURE UPPER BOUNDS ESTIMATES

The distance of $\mathbf{E}_0$ to $\Sigma_{[G]}$ is defined by

$$d(\mathbf{E}_0, \Sigma_{[G]}) = \min_{\mathbf{E}\in\Sigma_{[G]}} \|\mathbf{E}_0 - \mathbf{E}\|.$$

Estimates of the distance to a symmetry class are obtained as

$$M(\mathbf{E}_0, \Sigma_{[G]}) = \min_{\mathbf{E}\in S\subset\Sigma_{[G]}} \|\mathbf{E}_0 - \mathbf{E}\|,$$

i.e., as the minimum over a subset S of the considered symmetry stratum.

It satisfies thus

$$d(\mathbf{E}_0, \Sigma_{[G]}) \leq M(\mathbf{E}_0, \Sigma_{[G]}).$$

Examples: Gazis–Tadjbakhsh–Toupin (1963), Vianello (1997), Klimeš (2018), Stahn–Müller–Bertram (2020), Oliver-Leblond et al. (2021).

OUTLINE

1 Linear elasticity

2 Distance to a symmetry class

3 Upper bounds estimates rather than distances

4 Likely symmetry coordinate system
Upper bounds estimate of the distance to cubic symmetry

Natural coordinate system of a cubic elasticity tensor

Harmonic decomposition of $\mathbf{E}$ (Backus, 1970, Cowin, 1989, Baerheim, 1993):

$$\mathbf{E} = (\lambda, \mu, \mathbf{d}', \mathbf{v}', \mathbf{H}) \in \mathbb{H}^0 \oplus \mathbb{H}^0 \oplus \mathbb{H}^2 \oplus \mathbb{H}^2 \oplus \mathbb{H}^4$$

Let $\mathbf{E} = (\lambda, \mu, 0, 0, \mathbf{H}) \in \overline{\Sigma}_{[\mathbb{O}]}$ be a cubic elasticity tensor.

It has been shown (Abramian et al, 2020) that an orthotropic solution $\mathbf{a}'$ of the linear equation

$$\operatorname{tr}(\mathbf{H} \times \mathbf{a}) = \operatorname{tr}(\mathbf{H} \times \mathbf{a}') = 0, \qquad \mathbf{H} \times \mathbf{a} := -(\mathbf{a} \cdot \boldsymbol{\varepsilon} \cdot \mathbf{H})^s$$

provides the axes of symmetry $\langle \boldsymbol{e}_i \rangle$ of the cubic harmonic tensor $\mathbf{H} \in \Sigma_{[\mathbb{O}]}$.

$\mathbf{a}$ is not a covariant of $\mathbf{E}$.

LIKELY CUBIC/ORTHOTROPIC COORDINATE SYSTEM

In the spirit of Klimeš (2018) for transverse isotropy, equation $\operatorname{tr}(\mathbf{H} \times \mathbf{a}') = 0$ can be used to determine a likely cubic/orthotropic coordinate system.

Given a raw elasticity tensor

$$\mathbf{E}_0 = (\lambda_0, \mu_0, \mathbf{d}'_0, \mathbf{v}'_0, \mathbf{H}_0),$$

a likely cubic basis $(\boldsymbol{e}_1, \boldsymbol{e}_2, \boldsymbol{e}_3)$ for $\mathbf{E}_0$ is the eigenbasis of an orthotropic deviatoric second-order tensor $\mathbf{a}'$ which minimizes

$$\min_{\|\mathbf{a}'\|=1} \|\operatorname{tr}(\mathbf{H}_0 \times \mathbf{a}')\|^2, \qquad \mathbf{a}' \in \mathbb{H}^2.$$

Cubic elasticity upper bounds estimates

For any orthotropic second-order tensor **a**, we define

$$\mathbf{C}_{\mathbf{a}} := \sqrt{\frac{15}{2}} \frac{((\mathbf{a}^2 \times \mathbf{a}) \cdot (\mathbf{a}^2 \times \mathbf{a}))'}{\|\mathbf{a}^2 \times \mathbf{a}\|^2} \in \mathbb{H}^4, \qquad \|\mathbf{C}_{\mathbf{a}}\| = 1,$$

of cubic symmetry group $G_{\mathbf{C}_{\mathbf{a}}} \in [\mathbb{O}]$. We get a cubic tensor

$$\mathbf{E} = 2\mu_0 \mathbf{I} + \lambda_0 \mathbf{1} \otimes \mathbf{1} + (\mathbf{C}_{\mathbf{a}} :: \mathbf{H}_0)\, \mathbf{C}_{\mathbf{a}} \in \Sigma_{[\mathbb{O}]},$$

and define an upper bound estimate of $d(\mathbf{E}_0, [\mathbb{O}])$, as

$$\Delta_{\mathbf{a}}(\mathbf{E}_0, [\mathbb{O}]) = \|\mathbf{E}_0 - \mathbf{E}\|.$$

The Stahn et al (2020) cubic upper bound estimate is then simply recovered as

$$M(\mathbf{E}_0, [\mathbb{O}]) = \Delta_{\mathbf{t}_0}(\mathbf{E}_0, [\mathbb{O}]),$$

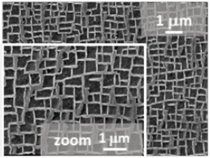
by setting $\mathbf{a} = \mathbf{t}_0 = \frac{2}{3}(\mathbf{d}_0 - \mathbf{v}_0) = \frac{2}{3}(\operatorname{tr}_{12} \mathbf{E}_0 - \operatorname{tr}_{13} \mathbf{E}_0)$.

EXAMPLE OF NI-BASED SUPERALLOY

Consider the elasticity tensor (in Kelvin representation)

$$[\mathbf{E}_0] = \begin{pmatrix} 243 & 136 & 135 & 22\sqrt{2} & 52\sqrt{2} & -17\sqrt{2} \\ 136 & 239 & 137 & -28\sqrt{2} & 11\sqrt{2} & 16\sqrt{2} \\ 135 & 137 & 233 & 29\sqrt{2} & -49\sqrt{2} & 3\sqrt{2} \\ 22\sqrt{2} & -28\sqrt{2} & 29\sqrt{2} & 133\cdot 2 & -10\cdot 2 & -4\cdot 2 \\ 52\sqrt{2} & 11\sqrt{2} & -49\sqrt{2} & -10\cdot 2 & 119\cdot 2 & -2\cdot 2 \\ -17\sqrt{2} & 16\sqrt{2} & 3\sqrt{2} & -4\cdot 2 & -2\cdot 2 & 130\cdot 2 \end{pmatrix} \text{GPa},$$

measured by François–Geymonat–Berthaud (1998) for a single crystal Ni-based superalloy with a so-called cubic γ/γ' microstructure (Fig. after Mattiello, 2018):



$d(\mathbf{E}_0, [\mathbb{O}])$		$M = \Delta_{\mathbf{t}_0}$	$\Delta_{\mathbf{d}_{20}}$	$\Delta_{\mathbf{a}'}$
74.13	Estimate (GPa):	241.7	238.6	114.9
0.1039^2	Relative estimate:	0.3388	0.3344	0.1610

Table: Comparison of upper bounds estimates of the distance to cubic elasticity $d(\mathbf{E}_0, [\mathbb{O}])$ for Ni-based single crystal superalloy.

The material considered has a cubic Ni-based microstructure.
All 2nd-order covariants of a cubic elasticity tensor are close to be isotropic.
They do not carry information about the cubic coordinate system.

[2] François et al (1998).

CLOSURE

- Possible accurate analytical estimation of the distance of a raw elasticity tensor $\mathbf{E}_0$ (ex. to cubic symmetry).
- Key point: the use of a second-order tensor **a** (not necessarily a covariant of $\mathbf{E}_0$), which carries the likely symmetry coordinate system.
- The optimal tensor $\mathbf{E}$, used to define an upper bound estimate as $\|\mathbf{E}_0 - \mathbf{E}\|$, is determined a priori. This allows to consider readily other norms than the Euclidean norm.

Log-Euclidean upper bounds estimates

For a given tensor $\mathbf{E}_0$, once an elasticity tensor $\mathbf{E}$ either cubic ($\mathbf{E} \in \Sigma_{[\mathbb{O}]}$) or orthotropic ($\mathbf{E} \in \Sigma_{[\mathbb{D}_2]}$) has been computed according to the symmetry group of a second-order tensor, say $\mathbf{a}$, one can easily calculate the upper bounds estimates $\Delta_{\mathbf{a}}(\mathbf{E}_0, \Sigma_{[G]})$ for any norm.

Since an elasticity tensor has to be positive definite, one can consider the Log-Euclidean norm (Arsigny et al, 2005, Moakher and Norris, 2006),

$$\|\mathbf{E}\|_L := \|\ln(\mathbf{E})\| = \|\ln([\mathbf{E}])\|_{\mathbb{R}^6},$$

which has the property of invariance by inversion.
For this norm, the upper bounds estimates of the distance

$$d(\mathbf{E}_0, \Sigma_{[G]}) = \min_{\Sigma_{[G]}} \|\mathbf{E}_0 - \mathbf{E}\|_L,$$

can then be expressed as

$$\Delta_{\mathbf{a}}(\mathbf{E}_0, \Sigma_{[G]}) := \|\mathbf{E}_0 - \mathbf{E}\|_L = \|\ln(\mathbf{E}_0) - \ln(\mathbf{E})\|.$$

Examples with Log-Euclidean norm (cubic symmetry)

	$\Delta_{\mathbf{t}_0}$	$\Delta_{\mathbf{d}_{20}}$	$\Delta_{\mathbf{a}'}$
Relative Euclidean estimate:	0.3388	0.3344	0.1610
Relative Log-Euclidean estimate:	0.1365	0.1353	0.0616

Table: Comparison of cubic upper bounds estimates for Ni-based single crystal superalloy.

The symmetry classes, their number, and their partial ordering are strongly dependent on the tensor type.

There are two symmetry classes for a vector $\mathbf{v}$:

- $[\mathrm{SO}(2)]$ (axial symmetry, if $\mathbf{v} \neq 0$)
- and $[\mathrm{SO}(3)]$ (isotropy, if $\mathbf{v} = 0$).

There are three symmetry classes for a symmetric second-order tensor $\mathbf{a}$ (and for a deviatoric tensor $\mathbf{a}'$):

- $[\mathbb{D}_2]$ (orthotropy, if $\mathbf{a}$ has three distinct eigenvalues),
- $[\mathrm{O}(2)]$ (transverse isotropy, if $\mathbf{a}$ has two distinct eigenvalues),
- and $[\mathrm{SO}(3)]$ (isotropy, if $\mathbf{a}' = 0$);

The symmetry classes for an harmonic (totally symmetric and traceless) fourth-order tensor $\mathbf{H}$ are the same eight symmetry classes as those of an elasticity tensor (Ihrig and Golubitsky, 1984, Forte and Vianello, 1996): $[\mathbb{1}]$, $[\mathbb{Z}_2]$, $[\mathbb{D}_2]$, $[\mathbb{D}_3]$, $[\mathbb{D}_4]$, $[\mathbb{O}]$, $[\mathrm{O}(2)]$ and $[\mathrm{SO}(3)]$ (isotropy, $\mathbf{H} = 0$).

Geometric consequences

1. the vector covariants $\mathbf{v}(\mathbf{E})$ of a monoclinic elasticity tensor $\mathbf{E}$ are all collinear,
2. the vector covariants $\mathbf{v}(\mathbf{E})$ of an elasticity tensor $\mathbf{E}$ either orthotropic, tetragonal, trigonal, cubic, transversely isotropic or isotropic, all vanish:

$$\mathbf{v}(\mathbf{E}) = 0 \quad \forall \mathbf{E} \in \Sigma_{[\mathbb{D}_2]} \cup \Sigma_{[\mathbb{D}_3]} \cup \Sigma_{[\mathbb{D}_4]} \cup \Sigma_{[\mathbb{O}]} \cup \Sigma_{[\mathrm{O}(2)]} \cup \Sigma_{[\mathrm{SO}(3)]},$$

3. the second-order covariants $\mathbf{c}(\mathbf{E})$ of an elasticity tensor either cubic or isotropic are all isotropic,
4. the second-order covariants $\mathbf{c}(\mathbf{E})$ of an elasticity tensor $\mathbf{E}$ either tetragonal, trigonal or transversely isotropic, of axis $\langle \boldsymbol{n} \rangle$, are all at least transversely isotropic of axis $\langle \boldsymbol{n} \rangle$,
5. the second-order covariants $\mathbf{c}(\mathbf{E})$ of an orthotropic elasticity tensor $\mathbf{E}$ are all at least orthotropic (and all of them commute with each other).
6. the second-order covariants $\mathbf{c}(\mathbf{E})$ of a triclinic elasticity tensor $\mathbf{E}$ are all at least orthotropic (but the natural basis may differ from one covariant to another).

Remark

Any other second-order covariant $\mathbf{c}(\mathbf{E}_0)$ of the elasticity tensor $\mathbf{E}_0$ can be added to the list $\{\mathbf{t}_0, \mathbf{d}_{20}, \mathbf{a}', \mathbf{b}'\}$, such as

$$\begin{array}{rrrrr} \mathbf{d}_0, & \mathbf{v}_0, & \mathbf{d}_0^2, & \mathbf{v}_0^2, & (\mathbf{d}_0\mathbf{v}_0)^s, \\ \mathbf{H}_0 : \mathbf{d}_0, & \mathbf{H}_0 : \mathbf{v}_0, & \mathbf{H}_0 : \mathbf{d}_0^2, & \mathbf{H}_0 : \mathbf{v}_0^2, & \mathbf{H}_0 : (\mathbf{d}_0\mathbf{v}_0)^s, \\ \mathbf{c}_3 = \mathbf{H}_0 : \mathbf{d}_{20}, & \mathbf{c}_4 = \mathbf{H}_0 : \mathbf{c}_3, & \mathbf{c}_5 = \mathbf{H}_0 : \mathbf{c}_4, & \dots & \end{array}$$

Explicit harmonic decomposition

The explicit harmonic decomposition of **E** is (Backus, 1970, Spencer, 1970)

$$\mathbf{E} = 2\mu\,\mathbf{I} + \lambda\,\mathbf{1}\otimes\mathbf{1} + \frac{2}{7}\,\mathbf{1}\odot(\mathbf{d}' + 2\mathbf{v}') + 2\,\mathbf{1}\otimes_{(2,2)}(\mathbf{d}' - \mathbf{v}') + \mathbf{H},$$

which can also be written as (Cowin, 1989, Baerheim, 1993)

$$\begin{aligned}\mathbf{E} =& 2\mu\,\mathbf{I} + \lambda\,\mathbf{1}\otimes\mathbf{1}\\ &+ \frac{1}{7}\Big(\mathbf{1}\otimes(5\mathbf{d}' - 4\mathbf{v}') + (5\mathbf{d}' - 4\mathbf{v}')\otimes\mathbf{1}\\ &\qquad + 2\,\mathbf{1}\,\underline{\overline{\otimes}}\,(6\mathbf{v}' - 4\mathbf{d}') + 2(6\mathbf{v}' - 4\mathbf{d}')\,\underline{\overline{\otimes}}\,\mathbf{1}\Big)\\ &+ \mathbf{H},\end{aligned}$$

where $\otimes_{(2,2)}$ is the Young-symmetrized tensor product,

$$\mathbf{a}\otimes_{(2,2)}\mathbf{b} = \frac{1}{3}\big(\mathbf{a}\otimes\mathbf{b} + \mathbf{b}\otimes\mathbf{a} - \mathbf{a}\,\underline{\overline{\otimes}}\,\mathbf{b} - \mathbf{b}\,\underline{\overline{\otimes}}\,\mathbf{a}\big),$$

$$(\mathbf{a}\,\underline{\overline{\otimes}}\,\mathbf{b})_{ijkl} := \frac{1}{2}(a_{ik}b_{jl} + a_{il}b_{jk}), \qquad I_{ijkl} = (\mathbf{1}\,\underline{\overline{\otimes}}\,\mathbf{1})_{ijkl} = \frac{1}{2}(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}).$$

The normal form $\mathbf{E}_{\mathbb{O}}$ of the cubic estimate $\mathbf{E}$ is obtained directly, as

$$[\mathbf{E}] = \begin{pmatrix} (\mathbf{E})_{1111} & (\mathbf{E})_{1122} & (\mathbf{E})_{1122} & 0 & 0 & 0 \\ (\mathbf{E})_{1122} & (\mathbf{E})_{1111} & (\mathbf{E})_{1122} & 0 & 0 & 0 \\ (\mathbf{E})_{1122} & (\mathbf{E})_{1122} & (\mathbf{E})_{1111} & 0 & 0 & 0 \\ 0 & 0 & 0 & 2(\mathbf{E})_{1212} & 0 & 0 \\ 0 & 0 & 0 & 0 & 2(\mathbf{E})_{1212} & 0 \\ 0 & 0 & 0 & 0 & 0 & 2(\mathbf{E})_{1212} \end{pmatrix},$$

in Kelvin matrix representation, with

$$(\mathbf{E}_{\mathbb{O}})_{1111} = 2\mu_0 + \lambda_0 - \frac{2}{\sqrt{30}}\mathbf{C}_{\mathbf{a}} :: \mathbf{H}_0,$$

$$(\mathbf{E}_{\mathbb{O}})_{1122} = \lambda_0 + \frac{1}{\sqrt{30}}\mathbf{C}_{\mathbf{a}} :: \mathbf{H}_0,$$

$$(\mathbf{E}_{\mathbb{O}})_{1212} = \mu_0 + \frac{1}{\sqrt{30}}\mathbf{C}_{\mathbf{a}} :: \mathbf{H}_0.$$