Second strain-gradient elasticity for centro-symmetric cubic materials

femto-st SCIENCES & TECHNOLOGIES

Matthias DEMONTEAUX[1], Juan De La FIGUERA[2], Nicolas AUFFRAY[3], Fabien AMIOT[1]

[1] FEMTO-ST, UMLP/CNRS, [2] CSIC/IQF, [3] IJLRDA, Sorbonne Université.

Problem

Second strain-gradient elasticity introduced by Mindlin [1] to describe surface effects, but restricted to isotropic materials because of complexity (18 constitutive parameters). Experimental approach :

- is very difficult for isotropic (amorphous) materials ;
- is already achieved for crystals, but no framework available to interpret.

Goal :
Optimal parametrization of second strain-gradient elasticity with cubic symmetry
$\mathcal{O} \times \mathrm{Z}_2$
(denoted as $m\bar{3}m$ in Hermann–Mauguin notation)

Constitutive law

$u : \Omega \subset \mathbb{R}^3 \longrightarrow \mathbb{R}^3$: displacement field on Ω. The free energy density depends on three state tensors :

$$\psi\left(\varepsilon^1, \varepsilon^2, \varepsilon^3\right) \quad (1)$$

- $\varepsilon^1 \in S^2(\mathbb{R}^3)$ is the usual small-strain tensor (dimension 6);
- $\varepsilon^2 = \nabla \otimes \nabla \otimes u \in S^2(\mathbb{R}^3) \otimes \mathbb{R}^3$ is an order 3 tensor, symmetric with respect to the 2 first indices (dimension 18);
- $\varepsilon^3 = \nabla \otimes \nabla \otimes \nabla \otimes u \in S^3(\mathbb{R}^3) \otimes \mathbb{R}^3$ is an order 4 tensor, symmetric with respect to the 3 first indices (dimension 30).

Generalized stresses are conjugate of the state tensors with respect to the energy density :

$$\tau^i = \frac{\partial \psi}{\partial \varepsilon^i} \quad (2)$$

Assuming that ψ is a second order polynomial :

$$\begin{bmatrix} \tau^1 \\ \tau^2 \\ \tau^3 \end{bmatrix} = \underbrace{\begin{bmatrix} E & M & C \\ M^t & A & O \\ C^t & O^t & B \end{bmatrix}}_{\mathcal{L}} \begin{bmatrix} \varepsilon^1 \\ \varepsilon^2 \\ \varepsilon^3 \end{bmatrix} + \underbrace{\begin{bmatrix} \alpha \\ \beta \\ \mathcal{T}_0 \end{bmatrix}}_{\mathcal{T}} \quad (3)$$

- Odd-order tensors vanish because of centro-symmetry
- α is usually zeroed by choosing the initial configuration

$$\begin{bmatrix} \tau^1 \\ \tau^2 \\ \tau^3 \end{bmatrix} = \begin{bmatrix} E & 0 & C \\ 0^t & A & 0 \\ C^t & 0^t & B \end{bmatrix} \begin{bmatrix} \varepsilon^1 \\ \varepsilon^2 \\ \varepsilon^3 \end{bmatrix} + \begin{bmatrix} 0 \\ 0 \\ \mathcal{T}_0 \end{bmatrix} \quad (4)$$

$\mathcal{T}_0$ is denoted as the cohesion tensor.

Explicit Clebsch-Gordan problem

As the material is assumed centro-symmetric, the sole rotations $\mathcal{O}$ leaving the cube unchanged are considered. U, V and W are irreducible representations of $\mathcal{O}$:

- Does W appear in the decomposition of $U \otimes V$?
- If yes, what is the multiplicity ?
- What is a basis for W?

Solution :

- Character formula [2] allows to split a given representation into irreducible representations
- Projection formula [2] is used to build a basis for W.

Contact :
fabien.amiot@femto-st.fr

Decomposition

1. Decompose the state tensors on a basis consistent with the material symmetries
   - $S^2(\mathbb{R}^3) : U = V = \mathbb{R}^3$
   - $S^2(\mathbb{R}^3) \otimes \mathbb{R}^3 : U$ irreducible representation of $S^2(\mathbb{R}^3)$, $V = \mathbb{R}^3$
   - $S^3(\mathbb{R}^3) \otimes \mathbb{R}^3 : U$ irreducible representation of $S^3(\mathbb{R}^3)$, $V = \mathbb{R}^3$
2. Build the constitutive tensors basis from the tensorial product of the decomposition of the state tensors, and build their basis using the projection formula.

Results

- Decomposition of state tensors on subspaces compatible with $\mathcal{O}$ has been obtained (projectors) ;
- $\mathcal{T}_0$ is in particular shown to depend on two cohesion moduli ;
- An orthogonal basis for the constitutive tensors is obtained :
  - E depends on 3 elastic moduli, A requires 11 parameters ;
  - C is described by 9 parameters, B depends on 26 parameters.

Surface relaxation

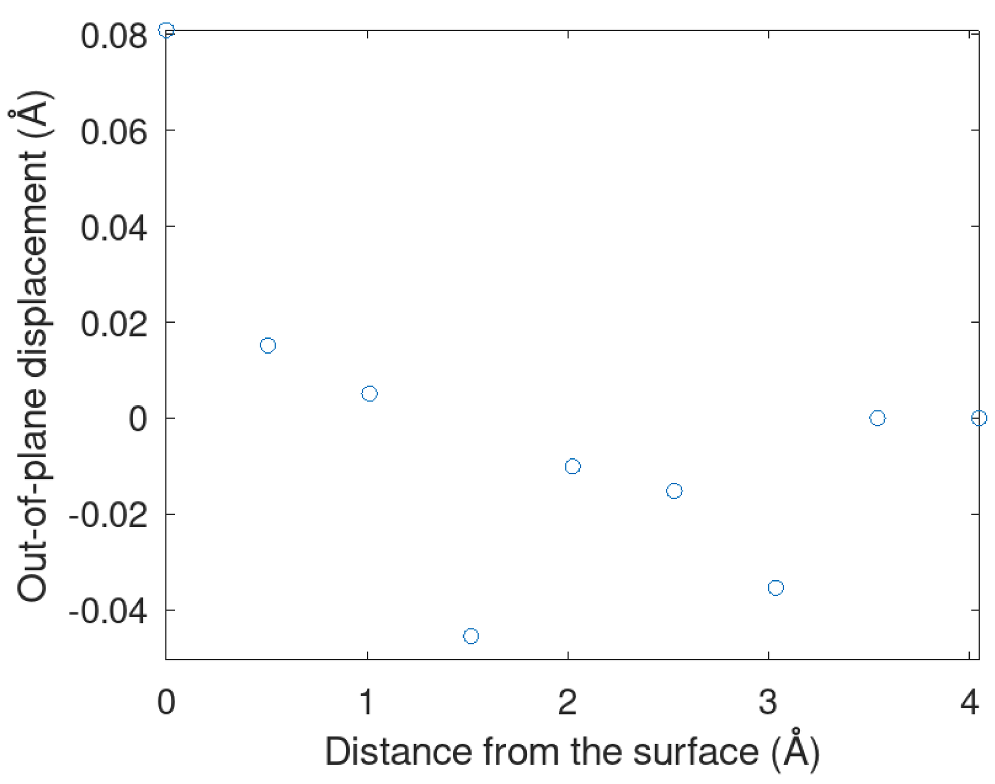
The surface relaxation problem is solved, considering a half-space, whose normal is x_1. For any crystal orientation, and for any displacement component u_i, the equilibrium imposes

$$\left(1 - l_{i1}^2 \frac{\mathrm{d}^2}{\mathrm{d}x_1^2}\right)\left(1 - l_{i2}^2 \frac{\mathrm{d}^2}{\mathrm{d}x_1^2}\right)\frac{\mathrm{d}^2 u_i}{\mathrm{d}x_1^2} = 0 \quad (5)$$

- The characteristic lengths l_{ij} are real or complex functions of the constitutive parameters and of the crystal orientation ;
- Only u_1 is nonzero because of the boundary conditions.

Low-energy electron diffraction (LEED)

- IV-LEED may be used to retrieve the surface structure of crystals
- Many surface structures, resulting from surface relaxation, have been compiled [3]. Ex : Cu(711) [4]



Conclusion

- Parametrization of second strain-gradient elasticity for centro-symmetric cubic materials
- Clear physical meaning of the parameters
- Towards the experimental identification of the parameters

Bibliography

[1] Mindlin, R. D. (1965). International journal of solids and structures, 1(4), 417-438.

[2] Fulton W., Harris J. (2013). Representation theory: a first course (Vol. 129). Springer Science & Business Media.

[3] Van Hove, M.A., Watson, P.R., Hermann, K.E. OSSD database. 1974-2004 https://www.fhi.mpg.de/1017073/oSSD

[4] Walter S. et al. (2001). Phys. Rev. B 63, 155407.

INSTITUT FEMTO-ST
15B avenue des Montboucons
25030 BESANÇON CEDEX
www.femto-st.fr