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RESEARCH ARTICLE

Toupin–Mindlin first strain-gradient elasticity for cubic and isotropic materials at small scales

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Abstract

The Toupin–Mindlin anisotropic first strain-gradient elasticity is a generalized continuum field theory valid at small scales. The field theoretical framework, the constitutive tensors, and the material parameters are given for anisotropic, cubic, and isotropic materials in first strain gradient elasticity. Since the characteristic lengths are in the unit-range of Ångström, first strain-gradient elasticity leads to Ångström mechanics, in a straightforward manner.

1 | INTRODUCTION

Strain-gradient elasticity and nonlocal elasticity theories are challenging generalized continuum theories to model crystals at small scales like the Ångström-scale (see, e.g., [1, 2]), where classical elasticity is not valid and leads to unphysical singularities. The theory of first strain-gradient elasticity in its modern form dates back to Toupin [3] and Mindlin [4]. Gradient elasticity has many advantages, since it provides a regularization based on higher-order partial differential equations and non-singular Green functions, and it possesses characteristic internal lengths able to describe size effects. For general anisotropic materials, the Toupin–Mindlin first strain-gradient elasticity contains three constitutive tensors. A mathematical modeling of the elastic properties of cubic crystals with centrosymmetry at small scales by means of the Toupin–Mindlin anisotropic first strain gradient elasticity theory has been given in Lazar et al. [2]. In this framework, two constitutive tensors are involved, a constitutive tensor of fourth-rank of the elastic constants and a constitutive tensor of sixth-rank of the gradient-elastic constants. The 14 material parameters (3 elastic and 11 gradient-elastic constants) and the corresponding three characteristic lengths are given. All material parameters of gradient elasticity can be determined from interatomic potentials. The numerical values of all material parameters are computed for aluminum as representative cubic material using a second nearest-neighbor modified embedded-atom-method (2NN MEAM) interatomic potential [2, 5]. Moreover, the isotropy conditions of first strain-gradient elasticity are given and discussed. A generalization of the Voigt average toward the sixth-rank constitutive tensor of the gradient-elastic constants is given in order to determine the five averaged isotropic gradient-elastic constants [2].

2 | TOUPIN–MINDLIN FIRST STRAIN-GRADIENT ELASTICITY

The Toupin–Mindlin first strain-gradient elasticity theory is an important generalized continuum theory of higher order. From a crystallographic point of view, crystals are anisotropic due to their crystal structure. Therefore, we consider first

the general anisotropic case and afterward, the cubic case. The isotropic case is also examined as an approximate case (see [2]).

2.1 | Field theoretical framework and general anisotropy

The *strain energy density* of anisotropic first strain-gradient elasticity theory reads

$$\mathcal{W}(\boldsymbol{e},\boldsymbol{\nabla e}) = \frac{1}{2}\,\mathbb{C}_{ijkl}e_{ij}e_{kl} + \mathbb{E}_{ijkln}e_{ij}\partial_n e_{kl} + \frac{1}{2}\,\mathbb{D}_{ijmkln}\partial_m e_{ij}\partial_n e_{kl}\,, \tag{1}$$

where e_{ij} is the *elastic strain tensor* which is given in terms of the *displacement vector* u_i:

$$e_{ij} = \frac{1}{2}\big(\partial_i u_j + \partial_j u_i\big)\,. \tag{2}$$

The partial derivative $\partial/\partial x_k$ with respect to the spatial coordinate x_k is denoted by ∂_k, and the indices run from 1 to 3, $i, j, k, l, m, n = 1, \dots, 3$. In Equation (1), there are three constitutive tensors $\mathbb{C}$, $\mathbb{E}$, and $\mathbb{D}$ of rank 4, 5, and 6, respectively, with the properties

- $\mathbb{C}$ has 21 independent components: $\mathbb{C}_{ijkl} \equiv \mathbb{C}_{(ij)|(kl)}$,
- $\mathbb{E}$ has 108 independent components: $\mathbb{E}_{ijklm} \equiv \mathbb{E}_{(ij)(kl)m}$,
- $\mathbb{D}$ has 171 independent components: $\mathbb{D}_{ijmkln} \equiv \mathbb{D}_{(ij)m|(kl)n}$.

Symmetrization over two indices is denoted by parenthesis, $A_{(ij)} := (A_{ij} + A_{ji})/2$, which indicates a minor symmetry and one vertical bar denotes the major symmetry as for $\mathbb{C}_{(ij)|(kl)}$ and $\mathbb{D}_{(ij)m|(kl)n}$. $\mathbb{E}_{(ij)(kl)m}$ does not possess any major symmetry, but only minor symmetries.

The *constitutive equations* for the *Cauchy stress tensor* $\boldsymbol{\sigma}$ and the *double stress tensor* $\boldsymbol{\tau}$ are given by

$$\sigma_{ij} = \frac{\partial \mathcal{W}}{\partial e_{ij}} = \mathbb{C}_{ijkl}e_{kl} + \mathbb{E}_{ijkln}\partial_n e_{kl}\,, \tag{3}$$

$$\tau_{ijm} = \frac{\partial \mathcal{W}}{\partial(\partial_m e_{ij})} = \mathbb{E}_{klijm}e_{kl} + \mathbb{D}_{ijmkln}\partial_n e_{kl}\,. \tag{4}$$

In the presence of body forces, the *Lagrangian density* reads

$$\mathcal{L} = -\mathcal{W} - \mathcal{V}\,, \tag{5}$$

where

$$\mathcal{V} = -f_i u_i \tag{6}$$

is the potential density of the body force density f_i. The *Euler–Lagrange equation* for first strain-gradient elasticity (or gradient elasticity of grade two with respect to the displacement field u_i) is given by

$$\frac{\delta \mathcal{L}}{\delta u_i} := \frac{\partial \mathcal{L}}{\partial u_i} - \partial_j \frac{\partial \mathcal{L}}{\partial(\partial_j u_i)} + \partial_m\partial_j \frac{\partial \mathcal{L}}{\partial(\partial_m\partial_j u_i)} = 0\,. \tag{7}$$

In terms of the Cauchy stress and double stress tensors, Equation (7) leads to the *force equilibrium condition* in first strain-gradient elasticity

$$\partial_j\big(\sigma_{ij} - \partial_m\tau_{ijm}\big) + f_i = 0\,. \tag{8}$$

Substituting the constitutive equations (3) and (4) and the elastic strain tensor (2) into the equilibrium condition (8), the following field equation for the displacement vector is obtained

$$L^{\mathrm{M}}_{ik}\,u_k = -f_i\,, \tag{9}$$

where

$$L^{\mathrm{M}}_{ik} = \mathbb{C}_{ijkl}\partial_j\partial_l + (\mathbb{E}_{ijklm} - \mathbb{E}_{klijm})\partial_j\partial_l\partial_m - \mathbb{D}_{ijmkln}\partial_j\partial_l\partial_m\partial_n \tag{10}$$

is the *Mindlin operator*, which is a linear differential operator of fourth order.

2.2 | Cubic crystals with centrosymmetry of point group $m\bar{3}m$

Important examples for cubic crystals with centrosymmetry of point group $m\bar{3}m$ are aluminum (Al), copper (Cu), iron (Fe), and tungsten (W). The three constitutive tensors of rank 4, 5, and 6, respecting minor and major symmetries, are given by [2]:

- The constitutive tensor of rank 4, $\mathbb{C}$, has three elastic constants, C_{11}, C_{12}, C_{44}, and reads

$$\mathbb{C}_{ijkl} = C_{12}\,\delta_{ij}\delta_{kl} + C_{44}\big(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}\big) + (C_{11} - C_{12} - 2C_{44})\,\delta_{ijkl} \tag{11}$$

  with

$$\delta_{ijkl} = \sum_{s=1}^{3} e_i^{(s)} e_j^{(s)} e_k^{(s)} e_l^{(s)}\,, \tag{12}$$

  where $\boldsymbol{e}^{(1)}$, $\boldsymbol{e}^{(2)}$, $\boldsymbol{e}^{(3)}$ are the (orthogonal) unit vectors of the cubic system.
- For crystals with centrosymmetry, the constitutive tensor of rank 5, $\mathbb{E}$, is zero: $\mathbb{E}_{ijkln} = 0$.
- The constitutive tensor of rank 6, $\mathbb{D}$, has 11 gradient-elastic constants, $a_1, \dots, a_{11}$, and reads

$$\begin{aligned}
\mathbb{D}_{ijmkln} = {} & \frac{a_1}{2}\big(\delta_{ij}\delta_{km}\delta_{ln} + \delta_{ij}\delta_{kn}\delta_{lm} + \delta_{kl}\delta_{im}\delta_{jn} + \delta_{kl}\delta_{in}\delta_{jm}\big) + 2a_2\,\delta_{ij}\delta_{kl}\delta_{mn} \\
& + \frac{a_3}{2}\big(\delta_{jk}\delta_{im}\delta_{ln} + \delta_{ik}\delta_{jm}\delta_{ln} + \delta_{il}\delta_{jm}\delta_{kn} + \delta_{jl}\delta_{im}\delta_{kn}\big) + a_4\big(\delta_{il}\delta_{jk}\delta_{mn} + \delta_{ik}\delta_{jl}\delta_{mn}\big) \\
& + \frac{a_5}{2}\big(\delta_{jk}\delta_{in}\delta_{lm} + \delta_{ik}\delta_{jn}\delta_{lm} + \delta_{jl}\delta_{km}\delta_{in} + \delta_{il}\delta_{km}\delta_{jn}\big) \\
& + a_6\big(\delta_{ik}\delta_{jlmn} + \delta_{il}\delta_{jkmn} + \delta_{jk}\delta_{ilmn} + \delta_{jl}\delta_{ikmn}\big) \\
& + a_7\big(\delta_{km}\delta_{ijln} + \delta_{lm}\delta_{ijkn} + \delta_{in}\delta_{jklm} + \delta_{jn}\delta_{iklm}\big) \\
& + a_8\,\delta_{mn}\delta_{ijkl} + a_9\big(\delta_{ij}\delta_{klmn} + \delta_{kl}\delta_{ijmn}\big) \\
& + a_{10}\big(\delta_{im}\delta_{jkln} + \delta_{jm}\delta_{ikln} + \delta_{kn}\delta_{ijlm} + \delta_{ln}\delta_{ijkm}\big) \\
& + a_{11}\,\delta_{ijklmn}
\end{aligned} \tag{13}$$

  with

$$\delta_{ijklmn} = \sum_{s=1}^{3} e_i^{(s)} e_j^{(s)} e_k^{(s)} e_l^{(s)} e_m^{(s)} e_n^{(s)}\,. \tag{14}$$

For cubic crystals with centrosymmetry of point group $m\bar{3}m$, the Mindlin operator (10) reduces to

$$\begin{aligned}
L^{\mathrm{M}}_{ik} = {} & (C_{12} + 2C_{44})\big[1 - \ell_1^2\Delta\big]\partial_i\partial_k + C_{44}\big[1 - \ell_2^2\Delta\big](\delta_{ik}\Delta - \partial_i\partial_k) \\
& + (C_{11} - C_{12} - 2C_{44})\big[1 - \ell_3^2\Delta\big]\delta_{ijkl}\partial_j\partial_l \\
& - a_6\,\delta_{ik}\delta_{jlmn}\partial_j\partial_l\partial_m\partial_n - a_{11}\delta_{ijklmn}\partial_j\partial_l\partial_m\partial_n \\
& - (a_6 + a_7 + a_9 + a_{10})(\delta_{klmn}\partial_i + \delta_{ilmn}\partial_k)\partial_l\partial_m\partial_n\,,
\end{aligned} \tag{15}$$

where it can be seen that it is given in terms of three *modified Helmholtz operators*

$$L_I = \left[1 - \ell_I^2 \Delta\right], \qquad I = 1, 2, 3 \tag{16}$$

with three *characteristic lengths* ℓ_I:

$$\ell_1^2 = \frac{2(a_1 + a_2 + a_3 + a_4 + a_5)}{C_{12} + 2C_{44}}, \tag{17}$$

$$\ell_2^2 = \frac{a_3 + 2a_4 + a_5}{2C_{44}}, \tag{18}$$

$$\ell_3^2 = \frac{a_6 + 2a_7 + a_8 + 2a_{10}}{C_{11} - C_{12} - 2C_{44}} \tag{19}$$

and three purely nonclassical parts given in terms of gradient-elastic constants.

2.3 | Atomistic representation of the constitutive tensors $\mathbb{C}$ and $\mathbb{D}$

In elasticity, the atomistic representation of the constitutive tensor $\mathbb{C}$ dates back to Born and Huang [6]. In first strain-gradient elasticity, the atomistic representation of the constitutive tensors of rank 4, 5, and 6 was given by Admal *et al.* [7]. The atomistic representation of the constitutive tensors $\mathbb{C}$ and $\mathbb{D}$ reads [6, 7]

$$\mathbb{C}_{ijkl} = \frac{1}{\Omega_\ell}\left[\frac{1}{4}\sum_{\substack{\alpha,\beta\\ \alpha\neq\beta}}\sum_{\substack{\gamma,\delta\\ \gamma\neq\delta}} \kappa^\ell_{\alpha\beta\gamma\delta}\frac{r_i^{\alpha\beta}r_j^{\alpha\beta}}{r^{\alpha\beta}}\frac{r_k^{\gamma\delta}r_l^{\gamma\delta}}{r^{\gamma\delta}} - \frac{1}{2}\sum_{\substack{\alpha,\beta\\ \alpha\neq\beta}}\varphi^\ell_{\alpha\beta}\frac{r_i^{\alpha\beta}r_j^{\alpha\beta}r_k^{\alpha\beta}r_l^{\alpha\beta}}{(r^{\alpha\beta})^3}\right], \tag{20}$$

$$\begin{aligned}\mathbb{D}_{ijmkln} = \frac{1}{\Omega_\ell}\Bigg[&\frac{1}{4}\sum_{\substack{\alpha,\beta\\ \alpha\neq\beta}}\sum_{\substack{\gamma,\delta\\ \gamma\neq\delta}} \kappa^\ell_{\alpha\beta\gamma\delta}\frac{r_i^{\alpha\beta}r_j^{\alpha\beta}r_k^{\gamma\delta}r_l^{\gamma\delta}}{r^{\alpha\beta}r^{\gamma\delta}}\frac{r_m^{\ell\alpha}+r_m^{\ell\beta}}{2}\frac{r_n^{\ell\gamma}+r_n^{\ell\delta}}{2}\\ &-\frac{1}{2}\sum_{\substack{\alpha,\beta\\ \alpha\neq\beta}}\varphi^\ell_{\alpha\beta}\frac{r_i^{\alpha\beta}r_j^{\alpha\beta}r_k^{\alpha\beta}r_l^{\alpha\beta}}{(r^{\alpha\beta})^3}\frac{r_m^{\ell\alpha}+r_m^{\ell\beta}}{2}\frac{r_n^{\ell\alpha}+r_n^{\ell\beta}}{2} + \frac{1}{2}\sum_{\substack{\alpha,\beta\\ \alpha\neq\beta}}\frac{\varphi^\ell_{\alpha\beta}}{r^{\alpha\beta}}G^{\alpha\beta\ell}_{pijm}G^{\alpha\beta\ell}_{pkln}\Bigg]\end{aligned} \tag{21}$$

with

$$\begin{aligned}G^{\alpha\beta\ell}_{pijm} = \frac{1}{2}\Bigg[&\delta_{pi}\left(r_j^{\alpha\beta}\frac{r_m^{\ell\alpha}+r_m^{\ell\beta}}{2} + r_m^{\alpha\beta}\frac{r_j^{\ell\alpha}+r_j^{\ell\beta}}{2}\right) + \delta_{pj}\left(r_i^{\alpha\beta}\frac{r_m^{\ell\alpha}+r_m^{\ell\beta}}{2} + r_m^{\alpha\beta}\frac{r_i^{\ell\alpha}+r_i^{\ell\beta}}{2}\right)\\ &-\delta_{pm}\left(r_i^{\alpha\beta}\frac{r_j^{\ell\alpha}+r_j^{\ell\beta}}{2} + r_j^{\alpha\beta}\frac{r_i^{\ell\alpha}+r_i^{\ell\beta}}{2}\right)\Bigg],\end{aligned} \tag{22}$$

where $\boldsymbol{r}^{\alpha\beta}$ is the vector connecting atom α to atom β and Ω_ℓ is the volume of the primitive lattice cell. The *bond force* $\varphi^\ell_{\alpha\beta}$ and the *bond stiffness* $\kappa^\ell_{\alpha\beta\gamma\delta}$ are defined by

$$\varphi^\ell_{\alpha\beta} = \frac{\partial \mathcal{V}^\ell}{\partial r^{\alpha\beta}} \qquad \text{and} \qquad \kappa^\ell_{\alpha\beta\gamma\delta} = \frac{\partial^2 \mathcal{V}^\ell}{\partial r^{\alpha\beta} r^{\gamma\delta}}, \tag{23}$$

where the *generic pair functional* reads

$$\mathcal{V}^\ell = \frac{1}{2}\sum_{\substack{\beta\\ \beta\neq\ell}}\phi(r^{\ell\beta}) + U(\rho^\ell), \tag{24}$$

with ϕ being the pair potential and U being the embedding function.

TABLE 1 Elastic constants for Al (fcc) computed from second nearest-neighbor modified embedded-atom-method (2NN MEAM) interatomic potential.

C_{11} [eV/Å^3]	C_{12} [eV/Å^3]	C_{44} [eV/Å^3]
0.71366	0.38649	0.19704

TABLE 2 Gradient-elastic constants for Al (fcc) computed from second nearest-neighbor modified embedded-atom-method (2NN MEAM) interatomic potential.

a_1 [eV/Å]	a_2 [eV/Å]	a_3 [eV/Å]	a_4 [eV/Å]	a_5 [eV/Å]	a_6 [eV/Å]
−0.02287	0.35854	-0.24815	0.16786	0.30012	0.08229
a_7 [eV/Å]	a_8 [eV/Å]	a_9 [eV/Å]	a_{10} [eV/Å]	a_{11} [eV/Å]	
−0.13198	−0.21058	−0.54849	0.41893	−0.19492	

TABLE 3 Characteristic lengths for Al (fcc) computed from second nearest-neighbor modified embedded-atom-method (2NN MEAM) interatomic potential.

ℓ_1 [Å]	ℓ_2 [Å]	ℓ_3 [Å]	a [Å]
1.19303	0.99186	2.58079 i	4.04950

2.4 | Numerical values of the material parameters using 2NN MEAM

In Toupin–Mindlin's first strain-gradient elasticity theory, the elastic constants and the gradient-elastic constants are characteristic material parameters which can be computed from interatomic potentials. Using the atomistic representation of the constitutive tensors $\mathbb{C}$ and $\mathbb{D}$, Equations (20) and (21), and the OpenKIM (Knowledgebase of Interatomic Models, E. Tadmor et al.) implementation of the 2NN MEAM interatomic potential, the material constants are computed (see [2, 5, 7]). For aluminum (Al), the numerical values of the 3 elastic constants, the 11 gradient-elastic constants, and the 3 characteristic lengths are given in Tables 1, 2, and 3, respectively, where a is the lattice constant. It is noticed that the 3 elastic constants given in Table 1 and the 11 gradient-elastic constants given in Table 2 satisfy the conditions for positive definiteness of $\mathcal{W}$ given in [2].

Using a Voigt representation in first strain gradient elasticity [2, 5, 7], the constitutive tensors of rank 4, $\mathbb{C}$, of elastic constants and rank 6, $\mathbb{D}$, of gradient-elastic constants can be represented as a symmetric (6×6) matrix and a symmetric (18×18) matrix, respectively. A graphical representation of them is given in Figure 1 for Al using the numerical values given in Tables 1 and 2 computed from 2NN MEAM interatomic potential.

2.5 | Isotropic first strain-gradient elasticity

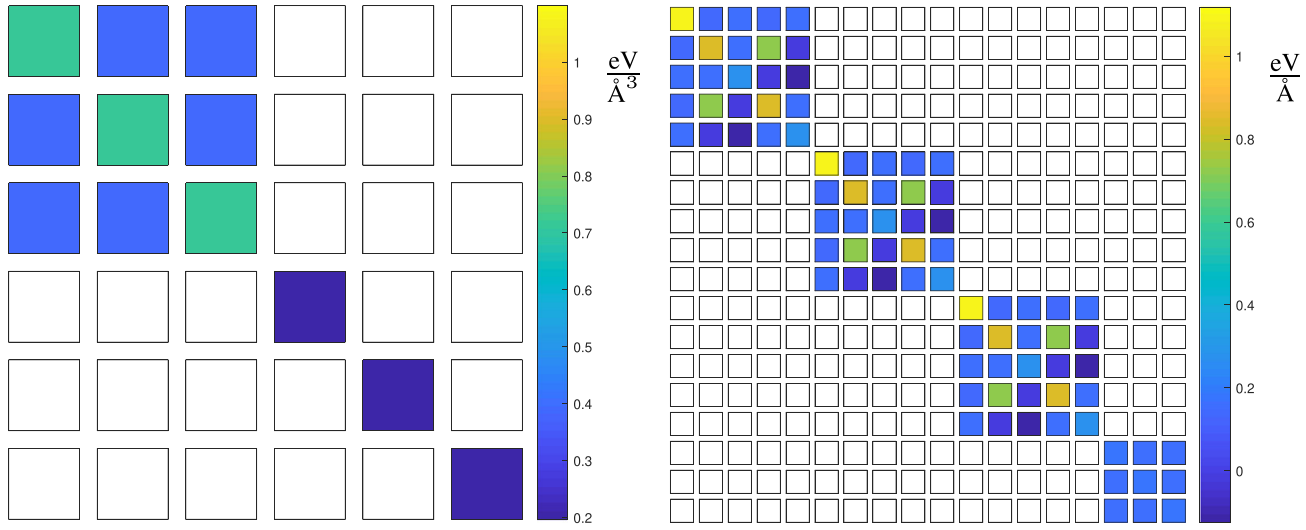
In the isotropic first strain-gradient elasticity, the constitutive tensors $\mathbb{C}$ and $\mathbb{D}$, respecting minor and major symmetries, are given by (see [2, 8–10]):

- The constitutive tensor of rank 4, $\mathbb{C}$, has two elastic constants and reads

$$\mathbb{C}_{ijkl} = \lambda\delta_{ij}\delta_{kl} + \mu\big(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}\big) \tag{25}$$

  with the two Lamé constants

$$\mu = C_{44} = \frac{1}{2}(C_{11} - C_{12})\,, \qquad \lambda = C_{12}\,. \tag{26}$$



(A) $\mathbb{C}$ for Al (2NN MEAM) (B) $\mathbb{D}$ for Al (2NN MEAM)

FIGURE 1 Voigt representation of the constitutive tensor $\mathbb{C}$ of elastic constants as (6×6) matrix and the constitutive tensor $\mathbb{D}$ of gradient-elastic constants as (18×18) matrix for Al (fcc) computed from second nearest-neighbor modified embedded-atom-method (2NN MEAM) interatomic potential.

- The constitutive tensor of rank 6, $\mathbb{D}$, has five gradient-elastic constants $a_1,\dots,a_5$ and reads

$$\begin{aligned}\mathbb{D}_{ijmkln} = {}& \frac{a_1}{2}\big(\delta_{ij}\delta_{km}\delta_{ln}+\delta_{ij}\delta_{kn}\delta_{lm}+\delta_{kl}\delta_{im}\delta_{jn}+\delta_{kl}\delta_{in}\delta_{jm}\big)+2a_2\,\delta_{ij}\delta_{kl}\delta_{mn}\\ &+\frac{a_3}{2}\big(\delta_{jk}\delta_{im}\delta_{ln}+\delta_{ik}\delta_{jm}\delta_{ln}+\delta_{il}\delta_{jm}\delta_{kn}+\delta_{jl}\delta_{im}\delta_{kn}\big)+a_4\big(\delta_{il}\delta_{jk}\delta_{mn}+\delta_{ik}\delta_{jl}\delta_{mn}\big)\\ &+\frac{a_5}{2}\big(\delta_{jk}\delta_{in}\delta_{lm}+\delta_{ik}\delta_{jn}\delta_{lm}+\delta_{jl}\delta_{km}\delta_{in}+\delta_{il}\delta_{km}\delta_{jn}\big)\,.\end{aligned} \tag{27}$$

For isotropic first strain-gradient elasticity, the Mindlin operator (10) reduces to

$$L^{\mathrm{M}}_{ik} = (\lambda+2\mu)\big[1-\ell_1^2\Delta\big]\partial_i\partial_k+\mu\big[1-\ell_2^2\Delta\big](\delta_{ik}\Delta-\partial_i\partial_k)\,, \tag{28}$$

where it can be seen that only two modified Helmholtz operators appear

$$L_I = \big[1-\ell_I^2\Delta\big]\,,\qquad I=1,2 \tag{29}$$

with two characteristic lengths ℓ_1 and ℓ_2:

$$\ell_1^2 = \frac{2(a_1+a_2+a_3+a_4+a_5)}{\lambda+2\mu}\,, \tag{30}$$

$$\ell_2^2 = \frac{a_3+2a_4+a_5}{2\mu}\,. \tag{31}$$

2.6 | Isotropy conditions

Comparing the constitutive tensor $\mathbb{C}$ for cubic crystals given in Equation (11) and for the isotropic case given in Equation (25), the isotropy condition for $\mathbb{C}$ reduces to

$$H = -(C_{11}-C_{12}-2C_{44}) = 0\,. \tag{32}$$

H is nothing but the anisotropy factor given by Hirth and Lothe [11]. Therefore, the isotropic condition for $\mathbb{C}$ means that the anisotropy factor must be zero. Next, comparing the constitutive tensor $\mathbb{D}$ for cubic crystals given in Equation (13) and

TABLE 4 Voigt-type averaged isotropic gradient-elastic constants and corresponding characteristic lengths for Al (fcc).

$\bar{a}_1$ [eV/Å]	$\bar{a}_2$ [eV/Å]	$\bar{a}_3$ [eV/Å]	$\bar{a}_4$ [eV/Å]	$\bar{a}_5$ [eV/Å]
−0.13862	0.22500	0.10877	0.15309	0.21632
$\bar{\ell}_1$ [Å]	$\bar{\ell}_2$ [Å]	$\bar{\ell}_1/a$	$\bar{\ell}_2/a$	a [Å]
1.20272	1.26566	0.2970	0.3125	4.04950

for the isotropic case given in Equation (27), the six isotropy conditions for $\mathbb{D}$ read

$$a_6 = a_7 = a_8 = a_9 = a_{10} = a_{11} = 0\,. \tag{33}$$

For aluminum, it holds: $H = 0.067$ and $a_6 = a_7 = a_8 = a_9 = a_{10} = a_{11} \neq 0$. Therefore, aluminum is nearly isotropic with respect to the 4th-rank constitutive tensor $\mathbb{C}$, but anisotropic with respect to the 6th-rank constitutive tensor $\mathbb{D}$. For that reason, an average is needed for the constitutive tensor of rank 6, $\mathbb{D}$, which is given in the next section.

2.7 | Voigt-type average of the 6th-rank constitutive tensor $\mathbb{D}$

For the calculation of the Voigt-type average of the 6th-rank constitutive tensor $\mathbb{D}$, its five linear invariants are used

$$I_1^{\mathbb{D}} = \mathbb{D}_{iijjkk}\,,\quad I_2^{\mathbb{D}} = \mathbb{D}_{iijkkj}\,,\quad I_3^{\mathbb{D}} = \mathbb{D}_{ijijkk}\,,\quad I_4^{\mathbb{D}} = \mathbb{D}_{ijkijk}\,,\quad I_5^{\mathbb{D}} = \mathbb{D}_{ijkjki}\,. \tag{34}$$

Based on the condition that the five linear invariants of the constitutive tensor of 6th-rank $\mathbb{D}_{ijmkln}$ representing the single cubic crystal must be equal to the linear invariants of the corresponding averaged isotropic 6th-rank constitutive tensor $\bar{\mathbb{D}}_{ijmkln}$, the following relations must hold:

$$I_1^{\mathbb{D}} = I_1^{\bar{\mathbb{D}}}\,,\qquad I_2^{\mathbb{D}} = I_2^{\bar{\mathbb{D}}}\,,\qquad I_3^{\mathbb{D}} = I_3^{\bar{\mathbb{D}}}\,,\qquad I_4^{\mathbb{D}} = I_4^{\bar{\mathbb{D}}}\,,\qquad I_5^{\mathbb{D}} = I_5^{\bar{\mathbb{D}}}\,. \tag{35}$$

The relations (35) provide the five *Voigt-type averaged isotropic gradient-elastic constants*, $\bar{a}_1, \ldots, \bar{a}_5$, in terms of the 11 gradient-elastic constants, $a_1, \ldots, a_{11}$, of the cubic crystal:

$$\bar{a}_1 = a_1 + \frac{2}{5}(a_7 + a_9 + a_{10}) + \frac{2}{35}a_{11}\,, \tag{36}$$

$$\bar{a}_2 = a_2 + \frac{1}{10}(a_8 + 2a_9) + \frac{1}{70}a_{11}\,, \tag{37}$$

$$\bar{a}_3 = a_3 + \frac{2}{5}(a_6 + 2a_{10}) + \frac{2}{35}a_{11}\,, \tag{38}$$

$$\bar{a}_4 = a_4 + \frac{1}{5}(2a_6 + a_8) + \frac{1}{35}a_{11}\,, \tag{39}$$

$$\bar{a}_5 = a_5 + \frac{2}{5}(a_6 + 2a_7) + \frac{2}{35}a_{11}\,. \tag{40}$$

Using the values given in Table 2, the numerical values for the five Voigt-type averaged isotropic gradient-elastic constants and the corresponding characteristic lengths are given in Table 4. It is noticed that the five averaged isotropic gradient-elastic constants given in Table 4 satisfy the conditions of positive definiteness of $\mathcal{W}$ given in [2] and the conditions of strong ellipticity given in [10].

3 | CONCLUSIONS

In this work, first strain-gradient elasticity has been presented as a generalized continuum field theory valid at small scales. For cubic materials of point group $m\bar{3}m$, Toupin–Mindlin's anisotropic first strain-gradient elasticity contains:

- 3 elastic constants

- 11 gradient-elastic constants
- 3 characteristic internal lengths.

On the other hand, Toupin–Mindlin's isotropic first strain-gradient elasticity contains:

- 2 elastic constants
- 5 gradient-elastic constants
- 2 characteristic internal lengths.

All material parameters can be computed from interatomic potentials like 2NN MEAM. A Voigt-type average is needed for the constitutive tensor of rank 6, $\mathbb{D}$, of the 5 isotropic gradient-elastic constants. The characteristic internal lengths are in the range of Ångström, which is the region where nonlocality is dominant. Therefore, strain-gradient elasticity leads to Ångström mechanics.

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