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Positive definiteness in coupled strain gradient elasticity

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Abstract The linear theory of coupled gradient elasticity has been considered for hemitropic second gradient materials, specifically the positive definiteness of the strain and strain gradient energy density, which is assumed to be a quadratic form of the strain and of the second gradient of the displacement. The existence of the mixed, fifth-rank coupling term significantly complicates the problem. To obtain inequalities for the positive definiteness including the coupling term, a diagonalization in terms of block matrices is given, such that the potential energy density is obtained in an uncoupled quadratic form of a modified strain and the second gradient of displacement. Using orthonormal bases for the second-rank strain tensor and third-rank strain gradient tensor results in matrix representations for the modified fourth-rank and the sixth-rank tensors, such that Sylvester's formula and eigenvalue criteria can be applied to yield conditions for positive definiteness. Both criteria result in the same constraints on the constitutive parameters. A comparison with results available in the literature was possible only for the special case that the coupling term vanishes. These coincide with our results.

Keywords Strain gradient elasticity · Coupling fifth-rank tensor · Positive definiteness of the potential energy

1 Introduction

The classical theory of elasticity is one of the most important tools of engineering suitable to describe many phenomena in bodies deformed under action of external forces. However, as any theory, it has a limited range of application. It is scale insensitive, and its solutions contain singularities when the boundary conditions contain singularities or the boundary geometry has sharp corners, as known from the Flamant–Boussinesq problem, the Kelvin problem, the crack tip problem and others [35]. Indeed, in order to take into account size effects (cf. [3,26,27]), to remove singularities in the stresses and displacements, when discontinues appear in the boundary conditions (e.g., [5,16,34,35]), to describe phenomena in the micro- and nanometer range like

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A natural generalization of classical elasticity is the strain gradient elasticity, in which higher derivatives of the displacement appear. An early work in this regard is [9], who introduced first the rotation gradient and the associated coupled stresses in the motion equations. The more general continua can be found almost fifty years later in [17,29,37]. These continua are called second gradient continua by [17] or strain gradient continua by [29], where the stored energy depends not only on the strain, but also on higher derivatives of the displacement field. It has been shown in various papers (cf. [15,24,25,32] among other) that some limitations of classical elasticity theory can be overcome with such gradient extensions.

Using the generalized mechanics incorporates higher gradients of the displacement leading to additional parameters effected by the inner structure at the microscale. Development of a general methodology for determining these additional parameters by using a computational approach was attempted in [1,2].

A key point of the theory is the uniqueness of the solution for the displacement field $\mathbf{u}(\mathbf{x})$ of the equilibrium equations. A necessary condition is the positive definiteness of the strain energy. The uniqueness proof for uncoupled isotropic gradient elasticity is due to [30]. Presuming that the constitutive coupling tensor \mathbb{C}_5 vanishes, this assumption leads to requirement of positive definiteness of both fourth-rank and sixth-rank constitutive tensors \mathbb{C}_4 and \mathbb{C}_6 . Inequality constrains on both constitutive parameters in the absence of coupling term are available in [11,19,29].

In the present paper, we extend the results of [11,30] and deduce the conditions of positive definiteness of stored elastic energy for coupled strain gradient elasticity. To do so, a block diagonalization of the composite stiffness in strain gradient elasticity is introduced. By this a formal diagonalization, which maps the constitutive fourth-, fifth- and a sixth-rank stiffness tensors \mathbb{C}_4 , \mathbb{C}_5 , \mathbb{C}_6 to a modified, decoupled representation involving \mathbb{C}_4 , \mathbb{C}_6^m , we give necessary conditions for positive definiteness, i.e. the convexity of the strain and strain gradient energy, involving the couple stiffness \mathbb{C}_5 .

The presentation is organized as follows: In the next section, we introduce notations used in the paper. Section 3 contains description of the block diagonalization of the composite stiffness in strain gradient elasticity which leads to the desired decoupling of the strain- and strain gradient parts in the strain energy density. In Sect. 4, the inequality constraints for all constitutive parameters are deduced using Sylvester's and positive eigenvalue criteria. The results are compared with the ones available in the literature for the special case that the coupling tensor \mathbb{C}_5 vanishes. The last section presents concluding remarks and a discussion.

2 Notation

Scalars, vectors, second- and higher-rank tensors are denoted by italic letters (like a or A), bold minuscules (like \mathbf{a}), bold majuscules (like \mathbf{A}) and blackboard bold majuscules (like \mathbb{A}), respectively.

The strain and strain gradient energy is

$$w = \frac{1}{2}\mathbf{H}_2 \cdot \mathbb{C}_4 \cdot \mathbf{H}_2 + \mathbf{H}_2 \cdot \mathbb{C}_5 \cdot \cdots \cdot \mathbb{H}_3 + \frac{1}{2}\mathbb{H}_3 \cdot \cdots \cdot \mathbb{C}_6 \cdot \cdots \cdot \mathbb{H}_3, \qquad (1)$$

where \mathbb{C}_4 , \mathbb{C}_5 , \mathbb{C}_6 are the stiffness tensors and the strains and the second gradient of displacement are defined as:

$$\mathbf{H}_2 = \frac{1}{2} (\mathbf{u} \otimes \nabla + \nabla \otimes \mathbf{u}), \qquad \mathbb{H}_3 = \mathbf{u} \otimes \nabla \otimes \nabla, \qquad (2)$$

which are calculated from the displacement field $\mathbf{u}(\mathbf{x})$, where \mathbf{x} is the position vector of a material point. For convenience, we drop the independent variable \mathbf{x} . " \otimes " denotes the dyadic product. ∇ is the nabla operator, with $\nabla_i = \frac{\partial}{\partial x_i} \mathbf{e}_i$, where \mathbf{e}_i denotes an orthonormal base vector. Repeated indices imply a summation. The nabla operator acts as follows on the displacement field \mathbf{u} :

$$\mathbf{u} \otimes \nabla = \frac{\partial u_i}{\partial x_j} \mathbf{e}_i \otimes \mathbf{e}_j = u_{i,j} \mathbf{e}_i \otimes \mathbf{e}_j \,. \tag{3}$$

The dots are scalar contractions of the form

$$\mathbf{v}_{1} \otimes \ldots \otimes \mathbf{v}_{k} \underbrace{\cdots}_{n \text{ dots}} \mathbf{w}_{l} \otimes \ldots \otimes \mathbf{w}_{l}$$
$$= (\mathbf{v}_{k-n} \cdot \mathbf{w}_{1}) \ldots (\mathbf{v}_{k} \cdot \mathbf{w}_{n}) \mathbf{v}_{1} \otimes \mathbf{v}_{k-n-1} \otimes \mathbf{w}_{n+1} \otimes \ldots \mathbf{w}_{l}.$$
(4)

For the double and triple scalar contractions in Eq. (1), the associations are

$$\mathbf{e}_{i} \otimes \mathbf{e}_{j} \cdot \mathbf{e}_{k} \otimes \mathbf{e}_{l} = \delta_{ik} \delta_{jl} , \qquad (5)$$

$$\mathbf{e}_{i} \otimes \mathbf{e}_{j} \otimes \mathbf{e}_{k} \cdots \mathbf{e}_{l} \otimes \mathbf{e}_{m} \otimes \mathbf{e}_{n} = \delta_{il} \delta_{jm} \delta_{kn} \,. \tag{6}$$

The arrangement of the scalar dot like : or \cdots has no implications. The stiffnesses for the case of hemitropy in accordance with [11,18,29] are

$$\mathbb{C}_{4} = \left[\lambda \delta_{ij} \delta_{kl} + \mu (\delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk})\right] \mathbf{e}_{i} \otimes \mathbf{e}_{j} \otimes \mathbf{e}_{k} \otimes \mathbf{e}_{l} \tag{7}$$

$$\mathbb{C}_{5} = \left[\kappa(\varepsilon_{imk}\delta_{jl} + \varepsilon_{ilk}\delta_{jm} + \varepsilon_{jmk}\delta_{il} + \varepsilon_{jlk}\delta_{im})\right]\mathbf{e}_{i} \otimes \mathbf{e}_{j} \otimes \mathbf{e}_{k} \otimes \mathbf{e}_{l} \otimes \mathbf{e}_{m}$$
(8)

$$\mathbb{C}_{6} = \begin{bmatrix} c_{1}(\delta_{jk}\delta_{im}\delta_{nl} + \delta_{jk}\delta_{in}\delta_{ml} + \delta_{ji}\delta_{kl}\delta_{mn} + \delta_{jl}\delta_{ik}\delta_{mn}) \\ + c_{2}(\delta_{ji}\delta_{km}\delta_{nl}\delta_{jm}\delta_{ki}\delta_{nl} + \delta_{ji}\delta_{kn}\delta_{ml} + \delta_{jn}\delta_{ik}\delta_{ml}) \\ + c_{3}(\delta_{jm}\delta_{kl}\delta_{in}\delta_{jl}\delta_{km} + \delta_{jn}\delta_{im}\delta_{kl} + \delta_{jl}\delta_{im}\delta_{nk}) \\ + c_{4}(\delta_{jn}\delta_{il}\delta_{km}\delta_{jm}\delta_{kn}\delta_{il}) \\ + c_{5}\delta_{il}\delta_{jk}\delta_{mn} \end{bmatrix} \mathbf{e}_{i} \otimes \mathbf{e}_{j} \otimes \mathbf{e}_{k} \otimes \mathbf{e}_{l} \otimes \mathbf{e}_{m} \otimes \mathbf{e}_{n}, \qquad (9)$$

where δ_{ij} is the Kronecker symbol and ε_{ijk} the Levi-Civita permutation symbol, λ and μ are Lamé's coefficients and κ and $c_{1...5}$ are the higher-order material parameters. One can check that the following index symmetries hold [19]

$$H_{ij} = H_{ji} \,, \tag{10}$$

$$H_{ijk} = H_{ikj},$$
(11)
$$G_{ijk} = G_{ijk}, G_{ijk},$$
(12)

$$C_{ijkl} = C_{klij} = C_{jikl} = C_{ijlk} , \qquad (12)$$

$$C_{ijklm} = C_{jiklm} = C_{ijkml} , \qquad (13)$$

$$C_{ijklmn} = C_{lmnijk} = C_{ikjlmn} = C_{ijklnm} , \qquad (14)$$

where the number of indices corresponds to the tensor rank of H_2 , \mathbb{H}_3 , \mathbb{C}_4 , \mathbb{C}_5 , \mathbb{C}_6 .

Remark 1 It is of no matter whether we consider $\mathbf{u} \otimes \nabla \otimes \nabla$ or $sym(\mathbf{u} \otimes \nabla) \otimes \nabla$ as the strain gradient. In both cases, we have a third-rank tensor with one index symmetry, which has 18 independent components. The linearized rotations that are purged from $\mathbf{u} \otimes \nabla$ upon symmetrization are replaced by additional compatibility conditions on \mathbb{H}_3 when $sym(\mathbf{u} \otimes \nabla) \otimes \nabla$ is used as the strain gradient.

Remark 2 Hemitropy implies that the material's symmetry group is the special orthogonal group SO(3), which is, loosely speaking, half the whole orthogonal group O(3) as in case of isotropy, which gives rise to the label "hemitropy." The absence of improper rotations preserves the existence of \mathbb{C}_5 , which is the only difference to isotropic strain gradient elasticity.

One can classify the subgroups of O(3) into three types:

- (1) Proper rotations with det(Q)=1 for all Q, where centro-symmetry is not included as it has det(-I)=-1
- (2) Improper rotations including the central inversion -I
- (3) Improper rotations excluding the central inversion -I

The absence of improper rotations implies absence of centro-symmetry. But the converse does not hold because of the existence of the third type of subgroups. The simplest example is the tetrahedral symmetry. A tetrahedron has rotational symmetries and mirror symmetries but no central inversion.

However, in case of isotropy in the sense that SO(3) is the symmetry group, adding a single mirror symmetry generates the whole of O(3), including centro-symmetry. Therefore, for isotropy it is sufficient to distinguish whether SO(3) or O(3) is the symmetry group, which can be reduced to asking whether the central inversion is part of the otherwise isotropic symmetry group. To differentiate these cases, one may call the case that O(3) represents all symmetries "isotropy" and the case that SO(3) represents all symmetries "hemitropy", where "hemi" refers to SO(3) being half of O(3), loosely speaking.

An example for a material that is hemitropic but not isotropic would be a body that is composed of chiral sub-bodies (for example tiny, left handed screw springs) that have an isotropic orientation distribution. On average, rotations do not change the structure, but a mirror operation flips the chirality of the springs.

3 Block diagonalization

It is known from Kirchhoff's uniqueness theorem [22,23] that in linear elasticity the conditions sufficient for a unique solution of the equilibrium equations for the displacement field require positive definiteness of the potential energy density w and a suppression of rigid body motions through appropriate boundary conditions. In second-gradient elasticity, the potential energy density is a quadratic form of strain \mathbf{H}_2 and second gradient of displacement \mathbb{H}_3 , see Eq. (1). The positive definiteness of w yields inequality constraints on stiffness tensors \mathbb{C}_4 , \mathbb{C}_5 and \mathbb{C}_6 .

For determination of these constrains, Eq. (1) can be rewritten in matrix form, and then, one of the criteria [20] (cf. Sylvester's criterion, positiveness of all matrix eigenvalues) should be applied to check the positive definiteness of w.

In the case that the coupling tensor \mathbb{C}_5 vanishes, w has a block diagonal form, which allows the independent determination of the constraints for the components of the tensors \mathbb{C}_4 and \mathbb{C}_6 . Such restrictions for the independent parameters μ and λ of \mathbb{C}_4 are standard in classical elasticity. Conditions for the positive definiteness of \mathbb{C}_6 were analyzed in [11,29].

The presence of the coupling tensor \mathbb{C}_5 significantly complicates the determination of conditions for positive definiteness of w. To decouple the strain and strain gradient contributions, we transform Eq. (1) by introducing a modified strain and second gradient of displacement:

$$w = \frac{1}{2}\mathbf{H}_{2}^{m} \cdot \mathbb{C}_{4} \cdot \mathbf{H}_{2}^{m} + \frac{1}{2}\mathbb{H}_{3} \cdots \mathbb{C}_{6}^{m} \cdots \mathbb{H}_{3}.$$
 (15)

Here the superscript m denotes the modified strains and the modified stiffness tensor. The modified stiffness tensor is specified as

$$\mathbb{C}_6^m = \mathbb{C}_6 - \mathbb{C}_5^T : \mathbb{C}_4^{-1} : \mathbb{C}_5.$$

$$(16)$$

Considering that the tensor \mathbb{C}_5 is symmetric with respect to the first two and to the last two indices $(C_{\underline{ijklm}})$, the transposition of \mathbb{C}_5 is $C_{\underline{ijklm}}^T = C_{\underline{klmij}}$, i.e. the first two and the last three entries are exchanged, \mathbf{H}_2 : $\mathbb{C}_5 \cdots \mathbb{H}_3 = \mathbb{H}_3 \cdots \mathbb{C}_5^T$: \mathbf{H}_2 . The modified strains are defined as

$$\mathbf{H}_{2}^{m} = \mathbf{H}_{2} + \mathbb{H}_{3} \cdots \mathbb{C}_{5}^{T} : \mathbb{C}_{4}^{-1} .$$

$$(17)$$

Inserting Eqs. (16) and (17) into Eq. (15) yields Eq. (1) upon summarizing.

Indeed, if Eq. (1) holds, the constitutive relations for the Cauchy stress and the double stress tensors are [33]

$$\mathbf{T}_2 = \frac{\partial w}{\partial \mathbf{H}_2} = \mathbb{C}_4 : \mathbf{H}_2 + \mathbb{C}_5 \cdots \mathbb{H}_3, \qquad (18)$$

$$\mathbb{T}_3 = \frac{\partial w}{\partial \mathbb{H}_3} = \mathbb{C}_5^T : \mathbf{H}_2 + \mathbb{C}_6 \cdots \mathbb{H}_3,$$
(19)

and for the modified form of w (Eq. 15), the constitutive relations have the same form:

$$\mathbf{T}_2 = \frac{\partial w}{\partial \mathbf{H}_2^m} = \mathbb{C}_4 : \mathbf{H}_2^m = \mathbb{C}_4 : \mathbf{H}_2 + \mathbb{C}_5 \cdots \mathbb{H}_3,$$
(20)

$$\mathbb{T}_3 = \frac{\partial w}{\partial \mathbb{H}_3} = \mathbb{C}_6^m \cdots \mathbb{H}_3 + \mathbb{C}_5^T : \mathbb{C}_4^{-1} : \mathbb{C}_4 \cdots \mathbf{H}_2^m = \mathbb{C}_5^T : \mathbf{H}_2 + \mathbb{C}_6 \cdots \mathbb{H}_3.$$
(21)

This is an additional validation of the block diagonalization.

Remark 3 We should point out that such a block diagonalization is applicable independently of the symmetry class of tensors.

In the case of hemitropy, the tensor \mathbb{C}_6^m is isotropic and is characterized by five derived constants

$$\mathbb{C}_{6}^{m} = \begin{bmatrix} c_{1}^{m} (\delta_{jk} \delta_{im} \delta_{nl} + \delta_{jk} \delta_{in} \delta_{ml} + \delta_{ji} \delta_{kl} \delta_{mn} + \delta_{jl} \delta_{ik} \delta_{mn}) \\ + c_{2}^{m} (\delta_{ji} \delta_{km} \delta_{nl} + \delta_{jm} \delta_{ki} \delta_{nl} + \delta_{ji} \delta_{kn} \delta_{ml} + \delta_{jn} \delta_{ik} \delta_{ml}) \\ + c_{3}^{m} (\delta_{jm} \delta_{kl} \delta_{in} + \delta_{jl} \delta_{in} \delta_{km} + \delta_{jn} \delta_{im} \delta_{kl} + \delta_{jl} \delta_{im} \delta_{nk}) \\ + c_{4}^{m} (\delta_{jn} \delta_{il} \delta_{km} + \delta_{jm} \delta_{kn} \delta_{il}) \\ + c_{5}^{m} \delta_{il} \delta_{ik} \delta_{mn} \Big] \mathbf{e}_{i} \otimes \mathbf{e}_{i} \otimes \mathbf{e}_{k} \otimes \mathbf{e}_{l} \otimes \mathbf{e}_{m} \otimes \mathbf{e}_{n},$$
(22)

where

$$c_1^m = c_1 - \frac{2\kappa^2}{\mu},$$
 (23)

$$c_2^m = c_2 + \frac{\kappa^2}{\mu},$$
 (24)

$$c_3^m = c_3 + \frac{2\kappa^2}{\mu},$$
 (25)

$$c_4^m = c_4 - \frac{4\kappa^2}{\mu},$$
 (26)

$$c_5^m = c_5 + \frac{4\kappa^2}{\mu} \,. \tag{27}$$

Remark 4 As mentioned above, the modified tensor \mathbb{C}_6^m is isotropic and is characterized by overall 7 parameters: the five independent parameters $c_1 - c_5$ in Eqs. (23)–(27) from the original \mathbb{C}_6 , the independent parameter κ in \mathbb{C}_5 , and μ , which is one of the Lamé constants of \mathbb{C}_4 . The other Lamé constant λ does not appear in \mathbb{C}_6^m . Indeed, the modified tensor \mathbb{C}_6^m is defined as a difference between the original tensor \mathbb{C}_6 and the contraction $\mathbb{C}_5^T : \mathbb{C}_4^{-1} : \mathbb{C}_5$. Examining this more closely, the λ drops out due to the contraction of the anti-symmetric Levi-Civita symbol with the symmetric Kronecker symbol in the term $\lambda \mathbf{I} \otimes \mathbf{I} = \lambda \delta_{ij} \delta_{kl} \mathbf{e}_i \otimes \mathbf{e}_j \otimes \mathbf{e}_k \otimes \mathbf{e}_l$. This is best seen in the projector representation of $\mathbb{C}_4^{-1} = (9K)^{-1}(\mathbf{I} \otimes \mathbf{I}) + (2\mu)^{-1}(\mathbb{I} - \frac{1}{3}\mathbf{I} \otimes \mathbf{I})$, with $\lambda = K - 2\mu/3$ and \mathbb{I} the identity on symmetric second-rank tensors. In \mathbb{C}_4^{-1} , only the first summand of the μ -part is nonzero upon carrying out the scalar contractions with \mathbb{C}_5^T and \mathbb{C}_5 .

The decoupling of the energy density simplifies determination of conditions for its positive definiteness. It yields a separation of inequality constraints on both tensors \mathbb{C}_4 and \mathbb{C}_6^m .

4 Positive definiteness of the elastic energy

For determining the inequality constraints for positive definiteness of \mathbb{C}_4 and \mathbb{C}_6^m , we rewrite Eqs. (15), (20), (21) in matrix form.

4.1 An orthonormal basis and matrix representations of strain gradient elasticity

In order to express the Cauchy stress \mathbf{T}_2 or the second-rank strain \mathbf{H}_2^m tensors as a 6-dimensional vector and write \mathbb{C}_4 as a 6 × 6 symmetric matrix, we use the following orthonormal basis vectors (for details see [6,7]):

$$\bar{\mathbf{e}}_p = \left(\frac{1-\delta_{ij}}{\sqrt{2}} + \frac{\delta_{ij}}{2}\right) (\mathbf{e}_i \otimes \mathbf{e}_j + \mathbf{e}_j \otimes \mathbf{e}_i), \ 1 \le p \le 6.$$
(28)

Then, the vectors $\boldsymbol{\tau}_2$, $\boldsymbol{\eta}_2^m$ and the matrix \mathbf{C}_4 can be written down in the form:

$$\boldsymbol{\tau}_2 = \sum_{p=1}^6 \overline{\boldsymbol{\tau}}_p \overline{\mathbf{e}}_p \,, \tag{29}$$

$$\boldsymbol{\eta}_2^m = \sum_{p=1}^6 \overline{\boldsymbol{\eta}}_p^m \overline{\mathbf{e}}_p \,, \tag{30}$$

$$\mathbf{C}_4 = \sum_{p,q=1}^6 \overline{C}_{pq} \overline{\mathbf{e}}_p \otimes \overline{\mathbf{e}}_q \,, \tag{31}$$

where the index ordering $i, j \rightarrow p$ is in accordance with the scheme of the Voigt notation [31,38],

$$1, 1 \to 1, 2, 2 \to 2, 3, 3 \to 3, 2, 3 \to 4, 1, 3 \to 5, 1, 2 \to 6.$$
(32)

With the new index running from 1 to 6, we have

$$\overline{\mathbf{e}}_p: \overline{\mathbf{e}}_q = \delta_{pq} \quad \text{with} \quad p, q = 1 \dots 6.$$
 (33)

This normalized basis has been used implicitly first by [36] and then made more explicit more than 100 years later by [28], see, e.g., [10]. An extensive account can be found in [8], chapter 26.

The third-rank double stress tensor \mathbb{T}_3 and the second gradient of displacement \mathbb{H}_3 can be represented w.r.t. the following orthonormal basis

$$\overline{\overline{\mathbf{e}}}_{\alpha} = \left(\frac{1-\delta_{ij}}{\sqrt{2}} + \frac{\delta_{ij}}{2}\right) \mathbf{e}_k \otimes (\mathbf{e}_i \otimes \mathbf{e}_j + \mathbf{e}_j \otimes \mathbf{e}_i), \ 1 \le \alpha \le 18,$$
(34)

as 18-dimensional vectors $\boldsymbol{\tau}_3$, $\boldsymbol{\eta}_3$

$$\boldsymbol{\tau}_{3} = \sum_{\alpha=1}^{18} \overline{\overline{\tau}}_{\alpha} \overline{\overline{\mathbf{e}}}_{\alpha} , \qquad (35)$$

$$\eta_3 = \sum_{\alpha=1}^{18} \overline{\overline{\eta}}_{\alpha} \overline{\overline{\mathbf{e}}}_{\alpha} , \qquad (36)$$

and the sixth-rank stiffness \mathbb{C}_6^m as a symmetric 18×18 matrix \mathbb{C}_6^m [6,7]:

$$\mathbf{C}_{6}^{m} = \sum_{\alpha,\beta=1}^{18} \overline{\overline{C}}_{\alpha\beta}^{m} \overline{\overline{\mathbf{e}}}_{\alpha} \otimes \overline{\overline{\mathbf{e}}}_{\beta}.$$
(37)

In the case of the three-to-one subscript, the correspondence $k, i, j \rightarrow \alpha$ is as follows:

Again we have orthogonality

$$\overline{\overline{\mathbf{e}}}_{\alpha} \cdots \overline{\overline{\mathbf{e}}}_{\beta} = \delta_{\alpha\beta} \quad \text{with} \quad \alpha, \beta = 1 \dots 18.$$
(39)

Remark 5 The double stresses \mathbb{T}_3 and the second gradient of displacement \mathbb{H}_3 are tensors of third-rank symmetric with respect to its last two indices. This is attributable to the form of the strain and strain gradient energy Eq. (1) and definition of the coupling tensor \mathbb{C}_5 .

With the orthonormal basis Eq. (28), the relationships between the vectors τ_2 , η_2^m and matrix components C_4 are

$$\overline{\tau}_p = \begin{cases} T_{ij} & \text{if } i = j ,\\ \sqrt{2} T_{ij} & \text{if } i \neq j , \end{cases}$$

$$\tag{40}$$

$$\overline{\eta}_p^m = \begin{cases} H_{ij}^m & \text{if } i = j ,\\ \sqrt{2} H_{ij}^m & \text{if } i \neq j , \end{cases}$$

$$\tag{41}$$

$$\overline{C}_{pq} = \begin{cases} C_{ijkl} & \text{if } i = j \text{ and } k = l ,\\ \sqrt{2} C_{ijkl} & \text{if } i \neq j \text{ and } k = l ,\\ 2 C_{ijkl} & \text{if } i \neq j \text{ and } k \neq l , \end{cases}$$
(42)

and with the orthonormal basis Eq. (34), the connection between the vectors τ_3 , η_3 and matrix components \mathbf{C}_6^m is

$$\overline{\overline{\tau}}_{\alpha} = \begin{cases} T_{kij} & \text{if } i = j ,\\ \sqrt{2} T_{kij} & \text{if } i \neq j , \end{cases}$$
(43)

$$\overline{\overline{\eta}}_{\alpha} = \begin{cases} H_{kij} & \text{if } i = j ,\\ \sqrt{2} H_{kij} & \text{if } i \neq j , \end{cases}$$
(44)

$$\overline{\overline{C}}_{\alpha\beta}^{m} = \begin{cases} C_{ijklmn}^{m} & \text{if } i = j \text{ and } l = m ,\\ \sqrt{2} C_{ijklmn}^{m} & \text{if } i \neq j \text{ and } l = m \text{ or } i = j \text{ and } l \neq m ,\\ 2 C_{ijklmn}^{m} & \text{if } i \neq j \text{ and } l \neq m . \end{cases}$$
(45)

Remark 6 The bar $\overline{\langle \ldots \rangle}$ above tensors and Latin subscripts p, g correspond to vectors and matrices with a two-to-one subscript transition, and the double bar $\overline{\overline{\langle \ldots \rangle}}$ above tensors and Greek indices α, β correspond to vectors and matrices with a three-to-one transition.

4.2 Application of Sylvester's criteria

We can now rewrite Eq. (15) in the matrix form

$$w = \frac{1}{2} (\eta_2^m)^T \mathbf{C}_4 \eta_2^m + \frac{1}{2} \eta_3^T \mathbf{C}_6^m \eta_3,$$
(46)

where η_2^m , C_4 , η_3 and C_6^m are defined by Eqs. (41)–(44), (45), (17), (16). Assume that the elastic energy density is a strictly convex function of the modified strain η_2^m and the second gradient of displacement η_3 , what is equivalent to the positive definiteness of the corresponding quadratic form Eq. (15). In the case of hemitropic materials (see Eqs. 7–9), the positive definiteness of w yields separate inequality constraints on both, the first and the second gradient constitutive parameters λ , μ , $c_{1...5}^m$. The standard Voigt representation for Cauchy stress and strain [38] yields the well-known constraints from classical mechanics for λ and μ

$$\mu > 0, \tag{47}$$

$$3\lambda + 2\mu > 0. \tag{48}$$

Next, we consider only the relationship between double stresses and the second gradient of displacement, which can be written as

$$\boldsymbol{\tau}_3 = \mathbf{C}_6^m \boldsymbol{\eta}_3,\tag{49}$$

where the matrix \mathbf{C}_6^m has following block diagonal form:

$$\mathbf{C}_{6}^{m} = \begin{pmatrix} \mathbf{C}^{(5)} & 0 & 0 & 0\\ 0 & \mathbf{C}^{(5)} & 0 & 0\\ 0 & 0 & \mathbf{C}^{(5)} & 0\\ 0 & 0 & 0 & \mathbf{C}^{(3)} \end{pmatrix}.$$
 (50)

Here 5 × 5 and 3 × 3 sub-matrices $C^{(5)}$, $C^{(3)}$ are specified

$$\mathbf{C}^{(5)} = \begin{pmatrix} a_1 & a_4 & a_5 & a_4 & a_5 \\ a_4 & a_2 & a_6 & 2c_2^m & \sqrt{2}c_1^m \\ a_5 & a_6 & a_3 & \sqrt{2}c_1^m & c_5^m \\ a_4 & 2c_2^m & \sqrt{2}c_1^m & a_2 & a_6 \\ a_5 & \sqrt{2}c_1^m & c_5^m & a_6 & a_3 \end{pmatrix},$$
(51)

$$\mathbf{C}^{(3)} = 2 \begin{pmatrix} c_4 & c_3 & c_3 \\ c_3^m & c_4^m & c_3^m \\ c_3^m & c_3^m & c_4^m \end{pmatrix},$$
(52)

with

$$a_1 = 4c_1^m + 4c_2^m + 4c_3^m + 2c_4^m + c_5^m, (53)$$

$$a_2 = 2c_2^m + 2c_3^m + 2c_4^m , (54)$$

$$a_3 = 2c_4^m + c_5^m \,, \tag{55}$$

$$a_4 = \sqrt{2(c_1^m + 2c_2^m)}, \qquad (56)$$

$$a_5 = 2c_1^m + c_5^m \,, \tag{57}$$

$$a_6 = \sqrt{2}(c_1^m + 2c_3^m) \,. \tag{58}$$

Remark 7 Neglecting the coupling tensor \mathbb{C}_5 in the constitutive Eqs. (18), (19), we obtain the results identical to one's presented in [11,38].

For the analysis of positive definiteness of the matrix \mathbb{C}_6^m , we apply the decomposition of the double stress \mathbb{T}_3 and of the second gradient of displacement \mathbb{H}_3 into a completely symmetric third-rank tensor and a deviatoric second-rank tensor

$$K_{kij} = \tilde{K}_{kij} + \frac{1}{3} (\varepsilon_{jkl} \hat{K}_{li} + \varepsilon_{ikl} \hat{K}_{lj}).$$
⁽⁵⁹⁾

Here \tilde{K}_{kij} is the completely symmetric part of \mathbb{K}_3 and \hat{K}_{li} is the sym-skew part of \mathbb{K}_3 , which are defined as

$$\tilde{K}_{kij} := \frac{1}{3} (K_{kij} + K_{ikj} + K_{ijk}),$$
(60)

$$\hat{K}_{li} := \varepsilon_{ljk} K_{kij} \,. \tag{61}$$

Using this decomposition, we can write down the constitutive Eq. (21) as follows (see [11,19])

$$\begin{pmatrix} \tilde{T}_{111} \\ \tilde{T}_{122} + \tilde{T}_{133} \\ \hat{T}_{32} - \hat{T}_{23} \end{pmatrix} = \mathbf{D}_{1}^{(3)} \begin{pmatrix} \tilde{H}_{111} \\ \tilde{H}_{122} + \tilde{H}_{133} \\ \hat{H}_{32} - \hat{H}_{23} \end{pmatrix} \begin{pmatrix} \tilde{T}_{222} \\ \tilde{T}_{233} + \tilde{T}_{112} \\ \hat{T}_{13} - \hat{T}_{31} \end{pmatrix} = \mathbf{D}_{1}^{(3)} \begin{pmatrix} \tilde{H}_{222} \\ \tilde{H}_{233} + \tilde{H}_{112} \\ \hat{H}_{13} - \hat{H}_{31} \end{pmatrix} \begin{pmatrix} \tilde{T}_{333} \\ \tilde{T}_{223} + \tilde{T}_{113} \\ \hat{T}_{21} - \hat{T}_{12} \end{pmatrix} = \mathbf{D}_{1}^{(3)} \begin{pmatrix} \tilde{H}_{333} \\ \tilde{H}_{223} + \tilde{H}_{113} \\ \hat{H}_{21} - \hat{H}_{12} \end{pmatrix} \end{cases} ,$$
(62)

$$\tilde{T}_{122} - \tilde{T}_{133} = 3d_2(\tilde{H}_{122} - \tilde{H}_{133}) \tilde{T}_{233} - \tilde{T}_{112} = 3d_2(\tilde{H}_{233} - \tilde{H}_{112}) \} ,$$
(63)

$$\tilde{T}_{223} - \tilde{T}_{113} = 3d_2(\tilde{H}_{223} - \tilde{H}_{113})$$

$$\hat{T}_{32} + \hat{T}_{23} = 6d_5(\hat{H}_{32} + \hat{H}_{23})$$

$$\hat{T}_{12} + \hat{T}_{23} = 6d_5(\hat{H}_{13} + \hat{H}_{23})$$

$$\hat{T}_{13} + \hat{T}_{31} = 6d_5(\hat{H}_{13} + \hat{H}_{31})$$

$$, \qquad (64)$$

$$\vec{T}_{21} + \vec{T}_{12} = 6d_5(\vec{H}_{21} + \vec{H}_{12})$$

$$\begin{pmatrix} I_{11} \\ \hat{T}_{22} \\ \hat{T}_{33} \end{pmatrix} = \mathbf{D}_2^{(3)} \begin{pmatrix} H_{11} \\ \hat{H}_{22} \\ \hat{H}_{33} \end{pmatrix} , \qquad (65)$$

$$\tilde{T}_{123} = 3d_2\tilde{H}_{123} \,. \tag{66}$$

Remark 8 The symbols $\langle \ldots \rangle$ and $\langle \ldots \rangle$ above a tensor in Eqs. (62)–(66) correspond to completely symmetric third-rank tensor and a deviatoric second-rank tensor.

The 3 \times 3 sub-matrices $\mathbf{D}_1^{(3)}, \mathbf{D}_2^{(3)}$ are specified as:

$$\mathbf{D}_{1}^{(3)} = \begin{pmatrix} d_{1} & 2d_{1} - d_{2} & d_{3} \\ 2d_{1} - d_{2} & 4d_{1} + d_{2} & 2d_{3} \\ d_{3} & 2d_{3} & d_{4} \end{pmatrix},$$
(67)

$$\mathbf{D}_{2}^{(3)} = d_{5} \begin{pmatrix} 2 & -1 & -1 \\ -1 & 2 & -1 \\ -1 & -1 & 2 \end{pmatrix},$$
(68)

where parameters $d_{1...5}$ are defined as

$$d_1 = 4c_1^m + 4c_2^m + 4c_3^m + 2c_4^m + c_5^m, (69)$$

$$d_2 = 2(c_4^m + 2c_3^m), (70)$$

$$d_3 = \frac{4}{3} (2c_2^m - c_1^m - c_5^m), \tag{71}$$

$$d_4 = \frac{8}{9} (2c_2^m + 3c_4^m + 2c_5^m - 4c_1^m - 3c_3^m),$$
(72)

$$d_5 = \frac{4}{9}(c_4^m - c_3^m), \tag{73}$$

Inserting Eqs. (23)-(27) into the latter equations gives

$$d_1 = 4c_1 + 4c_2 + 4c_3 + 2c_4 + c_5, (74)$$

$$d_2 = 2(c_4 + 2c_3), (75)$$

$$d_3 = \frac{4}{3}(2c_2 - c_1 - c_5), \tag{76}$$

$$d_4 = \frac{8}{9}(2c_2 + 3c_4 + 2c_5 - 4c_1 - 3c_3), \tag{77}$$

$$d_5 = \frac{4}{9}(c_4 - c_3 - \frac{6\kappa^2}{\mu}).$$
(78)

Thus, it turns out that only one of these d_i parameters, namely d_5 , is affected by the presence of the coupling tensor \mathbb{C}_5 .

Such a representation of constitutive relations between strain gradient and double stresses allows us to reduce the maximal dimension of coupled blocks to three. That enables us to apply the Sylvester's criteria [20]

to analyze the positive definiteness of the energy density. As a result, we obtain the following constraints for parameters $d_{1...5}$,

$$\begin{array}{c}
 d_1 > 0 \\
5d_5 > d_2 > 0 \\
 d_4 > \frac{5d_3^2}{5d_5 - d_2} \\
 d_5 > 0
\end{array}$$
(79)

what leads to constraints for constitutive parameters c_1 - c_5 , μ and κ

As mentioned above, if we take $\kappa = 0$, what implies the absence of coupling term \mathbb{C}_5 in the constitutive Eqs. (18), (19), these constraints are identical to the results presented by [11,29]. We consider this as an additional confirmation of Eq. (80).

For verification, we present another way of obtaining these inequalities in the next subsection, namely by extracting the eigenvalues of the \mathbb{C}_6^m symbolically with the aid of a computer algebra system and requiring their positivity. We apply the scheme proposed in [18] for the isotropic stiffness hexadic that appears in strain gradient elasticity.

4.3 Eigenvalues of the modified hexadic \mathbb{C}_6^m

In this section, we deduce conditions for positive definiteness of 18×18 matrix \mathbb{C}_6^m using eigenvalue technique. In accordance with these criteria, a matrix is positive definite if all its eigenvalues are positive.

It is shown in [18] that an isotropic hexadic with five independent parameters $c_1 - c_5$ has four distinct eigenvalues. Its spectral representation is

$$\mathbb{C}_6 = \sum_{i=1}^4 \lambda_i \mathbb{P}_i \,. \tag{81}$$

The projectors $\mathbb{P}_{1...4}$ are defined as

$$\mathbb{P}_1 = \overline{\mathbb{B}}_1 \,, \tag{82}$$

$$\mathbb{P}_2 = \overline{\mathbb{B}}_2 \,, \tag{83}$$

$$\mathbb{P}_{3} = \frac{1}{2} \left\{ \overline{\mathbb{B}}_{5} + \left[\frac{(12c_{1} - 16c_{2} + 2c_{3} + 9c_{5})}{6c_{r}} \overline{\mathbb{B}}_{3} + \frac{2\sqrt{5}(3c_{1} + 2c_{2} + 2c_{3})}{3c_{r}} \overline{\mathbb{B}}_{4} \right] \right\},$$
(84)

$$\mathbb{P}_{4} = \frac{1}{2} \left\{ \overline{\mathbb{B}}_{5} - \left[\frac{(12c_{1} - 16c_{2} + 2c_{3} + 9c_{5})}{6c_{r}} \overline{\mathbb{B}}_{3} + \frac{2\sqrt{5}(3c_{1} + 2c_{2} + 2c_{3})}{3c_{r}} \overline{\mathbb{B}}_{4} \right] \right\}$$
(85)

with respect to the basis

$$\overline{\mathbb{B}}_1 = -\frac{1}{15} \left(\mathbb{B}_1 + \mathbb{B}_2 + \mathbb{B}_5 \right) + \frac{1}{6} \left(\mathbb{B}_3 + \mathbb{B}_4 \right), \tag{86}$$

$$\overline{\mathbb{B}}_{2} = \frac{1}{12} \left(2 \,\mathbb{B}_{1} - \mathbb{B}_{2} - 2 \,\mathbb{B}_{3} + 4 \,\mathbb{B}_{4} - 4 \,\mathbb{B}_{5} \right), \tag{87}$$

$$\overline{\mathbb{B}}_{3} = \frac{1}{60} (6 \,\mathbb{B}_{1} - 9 \,\mathbb{B}_{2} + 16 \,\mathbb{B}_{5}), \qquad (88)$$

$$\overline{\mathbb{B}}_4 = \frac{1}{6\sqrt{5}} \left(3 \,\mathbb{B}_1 - 4 \,\mathbb{B}_5 \right),\tag{89}$$

$$\overline{\mathbb{B}}_5 = \frac{1}{20} (-2 \,\mathbb{B}_1 + 3 \,\mathbb{B}_2 + 8 \,\mathbb{B}_5) \,. \tag{90}$$

Here $\overline{\mathbb{B}}_{1...5}$ are linear combination of five base hexadics with components

$$B_{1\ ijklmn} = \delta_{jk}\delta_{im}\delta_{nl} + \delta_{jk}\delta_{in}\delta_{ml} + \delta_{ji}\delta_{kl}\delta_{mn} + \delta_{jl}\delta_{ik}\delta_{mn} , \qquad (91)$$

$$B_{2 \ ijklmn} = \delta_{ji} \delta_{km} \delta_{nl} + \delta_{jm} \delta_{ki} \delta_{nl} + \delta_{ji} \delta_{kn} \delta_{ml} + \delta_{jn} \delta_{ik} \delta_{ml} , \qquad (92)$$

$$B_{3\ ijklmn} = \delta_{jm} \delta_{kl} \delta_{in} + \delta_{jl} \delta_{in} \delta_{km} + \delta_{jn} \delta_{im} \delta_{kl} + \delta_{jl} \delta_{im} \delta_{nk} , \qquad (93)$$

$$\mathcal{B}_{4\ ijklmn} = \delta_{jn}\delta_{il}\delta_{km} + \delta_{jm}\delta_{kn}\delta_{il}\,,\tag{94}$$

$$B_{5\ ijklmn} = \delta_{il}\delta_{jk}\delta_{mn} \tag{95}$$

with respect to the basis { $\mathbf{e}_i \otimes \mathbf{e}_j \otimes \mathbf{e}_k \otimes \mathbf{e}_l \otimes \mathbf{e}_m \otimes \mathbf{e}_n$ }. The eigenvalues are linear combination of five independent parameters $c_{1...5}$,

$$A_1 = 2 \left(c_4 - c_3 \right), \tag{96}$$

$$\lambda_2 = 4 \, c_3 + 2 \, c_4 \,, \tag{97}$$

$$\lambda_3 = \frac{1}{2} (4 c_1 + 8 c_2 + 2 c_3 + 4 c_4 + 3 c_5) + c_r , \qquad (98)$$

$$\lambda_4 = \frac{1}{2} (4 c_1 + 8 c_2 + 2 c_3 + 4 c_4 + 3 c_5) - c_r$$
(99)

with

$$c_r = \sqrt{\frac{1}{36} \left(12 c_1 - 16 c_2 + 2 c_3 + 9 c_5\right)^2 + \frac{20}{9} \left(3 c_1 + 2 c_2 + 2 c_3\right)^2}.$$
 (100)

Introducing the dimensionless parameter γ as

$$\cos \gamma = \frac{(12c_1 - 16c_2 + 2c_3 + 9c_5)}{6c_r} \iff \sin \gamma = \frac{2\sqrt{5}(3c_1 + 2c_2 + 2c_3)}{3c_r}, \quad (101)$$

allows to use the four eigenvalues λ_1 , λ_2 , λ_3 , λ_4 and the parameter γ as the five independent parameters of \mathbb{C}_6 , where γ determines the third and fourth eigenprojector.

Using Eqs. (96)–(99), we can determine eigenvalues of the modified stiffness tensor \mathbb{C}_6^m in terms of $c_1^m - c_5^m$. It turns out that only λ_1 is altered by the presence of κ ,

$$\lambda_1^m = \lambda_1 - \frac{12\kappa^2}{\mu},\tag{102}$$

$$\lambda_{2...4}^m = \lambda_{2...4}.$$
 (103)

Since μ is itself an eigenvalue that is greater than zero, and κ^2 is also greater than zero, the presence of the coupling tensor \mathbb{C}_5 can only lower the eigenvalues, compared to the isotropic case. However, the eigenvalues cannot be interpreted directly physically or compared to the isotropic case, as the modification involves a modified strain \mathbf{H}_2^m . Nevertheless, one can check the sign, and notice that a too large magnitude of κ can always produce a negative λ_1^m and hence leads to an indefinite strain energy w.

Requiring positivity of the eigenvalues involving coupling tensor \mathbb{C}_5 , we obtain identical constraints for constitutive parameters $c_1 - c_5$, μ and κ as in Eq. (80).

5 Concluding remarks

Positive definiteness conditions for the quadratic strain and strain gradient energy for the linear theory of coupled gradient elasticity have been given for a hemitropic material. The presence of the coupling term \mathbb{C}_5 significantly complicates the problem. To avoid this complication, a transformation of the equation for the potential energy density Eq. (1) is made to represent w as an uncoupled quadratic form of the modified strain and second gradient of displacement Eq. (15). This transformation, effectively a block diagonalization, leads to decoupling of the strain and strain gradient term in the potential energy density. Further, introducing

orthonormal bases for the fourth- and sixth order tensors gives matrix representations for these tensors, which makes it possible to apply Sylvester's criteria and eigenvalue extraction. We obtain the same constraints in both cases. To the best of the authors knowledge, these results are not available in the literature and a comparison is possible only for the special case when the coupling tensor \mathbb{C}_5 vanishes. In this case, conditions for positive definiteness of the potential energy density are identical with ones presented in [11,29].

We found that in the case of hemitropic materials only one of the inequality constraints for the constitutive parameters $c_{1...5}$ and κ Eq. (80) is affected by presence of coupling tensor \mathbb{C}_5 . Due to the coupling, also the shear modulus μ appears when requiring positive definiteness of the sixth-rank stiffness. It turns out that large magnitudes of κ , i.e., strong coupling between strain and strain gradient, can always lead to indefinite elastic energies. We believe that the results presented in this work are the first of their type, both in terms of the block diagonal quadratic form of the potential energy density, which contains a coupling tensor \mathbb{C}_5 , and in terms of positive definiteness conditions for constitutive parameters.

As mentioned above, the block diagonalization is applicable independently of the symmetry class of materials and can be employed to anisotropic second gradient materials. However, a calculation by hand is hardly feasible. Instead, one needs to resort to computer algebra systems. For this purpose, we provide a notebook in the supplementary material.

Maybe even more important, the diagonalization opens the door to formally invert Hooke's law even in the coupled case. Due to the block diagonalization and the block matrix representations, one can easily obtain the coupled compliance tensors S_4 , S_5 , S_6 by forward modification $\{\mathbb{C}_4, \mathbb{C}_5, \mathbb{C}_6\} \rightarrow \{\mathbb{C}_4, \mathbb{C}_6^m\}$, inversion of the latter $\{\mathbb{C}_4, \mathbb{C}_6^m\} \rightarrow \{\mathbb{S}_4, \mathbb{S}_6^m\}$ and reversing the modification $\{\mathbb{S}_4, \mathbb{S}_6^m\} \rightarrow \{\mathbb{S}_4, \mathbb{S}_5, \mathbb{S}_6\}$. This allows finally for an explicit expression of the complementary energy even in the coupled case. This is prerequisite for generalizing various proofs from classical elasticity, which have not yet been given for gradient elasticity, like existence and uniqueness of solutions of boundary value problems with displacement or mixed boundary conditions.

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