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Gradient elasticity and nonstandard boundary conditions

Castrenze Polizzotto *

Department of Structural Engineering and Geotechnics, DISeG University of Palermo, Viale delle Scienze, 90128 Palermo, Italy

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Abstract

Gradient elasticity for a second gradient model is addressed within a suitable thermodynamic framework apt to account for nonlocality. The pertinent thermodynamic restrictions upon the gradient constitutive equations are derived, which are shown to include, besides the field (differential) stress–strain laws, a set of nonstandard boundary conditions. Consistently with the latter thermodynamic requirements, a surface layer with membrane stresses is envisioned in the strained body, which together with the above nonstandard boundary conditions make the body constitutively insulated (i.e. no long distance energy flows out of the boundary surface due to nonlocality). The total strain energy is shown to include a bulk and surface strain energy. A minimum total potential energy principle is provided for the related structural boundary-value problem. The Toupin–Mindlin polar-type strain gradient material model is also addressed and compared with the above one, their substantial differences are pointed out, particularly for what regards the constitutive equations and the boundary conditions accompanying the solving displacement equilibrium equations. A gradient one-dimensional bar sample in tension is considered for a few applications of the proposed theory.

Keywords: Nonlocal continua; Gradient elasticity; Boundary conditions

1. Introduction

In the 1960s, within the framework of polar and multipolar continua, the so-called strain-gradient elasticity theories, Truesdell and Toupin (1960), Toupin (1962), particularly in their linearized forms, Mindlin (1964, 1965), Mindlin and Eshel (1968), Green and Rivlin (1964), were most popular. In the latter theories, the material strain state is described by a set of $n+1$ strain tensors, say $\boldsymbol{\varepsilon}^{(v)}$ $(v = 0, 1, \ldots, n)$, in which $\boldsymbol{\varepsilon}^{(0)}$ identifies with the usual (small, second-order) strain tensor $\boldsymbol{\varepsilon}$ $(\boldsymbol{\varepsilon}^{(0)} \equiv \boldsymbol{\varepsilon})$, and the other $\boldsymbol{\varepsilon}^{(v)}$ are higher order strain tensors defined as spatial gradients either of the displacement field, that is

$$\boldsymbol{\varepsilon}^{(v)} = \nabla^v \nabla^s \mathbf{u} \quad (v = 1, 2, \ldots, n) \tag{1}$$

or of the strain field, that is

$$\boldsymbol{\varepsilon}^{(v)} = \nabla^v \boldsymbol{\varepsilon} \quad (v = 1, 2, \ldots, n), \tag{2}$$

* Tel.: +39-91-6568-411; fax: +39-91-6568-407.
E-mail address: cpoli@diseg.unipa.it (C. Polizzotto).

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where $\nabla^\nu := \{\partial_{i_1}\partial_{i_2}\ldots\partial_{i_\nu}\}$ is the νth-order gradient and ∇^s the symmetric part of ∇. Analogously, the related stress state is described by a set of $n+1$ stress tensors, say $\boldsymbol{\sigma}^{(\nu)}$ $(\nu = 0, 1, \ldots, n)$, which are work-conjugate of the $\boldsymbol{\varepsilon}^{(\nu)}$ and $\boldsymbol{\sigma}^{(0)}$ identifies with the usual (Cauchy) stress tensor.

At the constitutive level, however, the differential relations (1), or (2), are ignored, and the strain tensors, $\boldsymbol{\varepsilon}^{(\nu)}$, are all considered independent of one another, what seems appropriate for an adequate description of the deformation capabilities of a continuum simulating a particulate microstructure. In this way, the material strain and stress states are *locally* described by the two above sets of strain and stress tensors, namely $\boldsymbol{\varepsilon}^{(\nu)}$ and $\boldsymbol{\sigma}^{(\nu)}$ $(\nu = 0, 1, \ldots, n)$, and, under certain (stability) conditions, there is a one-to-one stress–strain correspondence. This implies that the gradient theory in question—though, as a special polar continuum theory, is endowed with one or more internal length parameters—proves to be a local theory in the sense that the stress state at a point depends only on the strain state at the same point, like for the classical Hookean theory.

Main research issues inherent in the aforementioned (Toupin–Mindlin) gradient elasticity theory were the correct way to write the displacement equilibrium equations and the related boundary conditions (to this purpose, the *compatibility* relations (1) played a crucial role), as well as the assessment of the appropriate multipolar body and surface forces constituting the loading data in the relevant boundary-value problem. Of particular interest was the formulation of the *extra* boundary conditions required by the higher order partial differential equations (PDEs) governing the problem, Mindlin (1964, 1965), Mindlin and Eshel (1968), Wu (1992).

It is worth observing that these extra boundary conditions play, within the gradient elasticity theory in question, the same role as the other boundary conditions, that is, as the standard boundary conditions in the classical Hookean boundary value-problem. Their purpose is in fact that of introducing the boundary data into the problem formulation, as a rule through an *alternative* as follows: *at every point of the boundary surface, either a (polar) force, or the work-conjugate displacement, is to be specified.* Mindlin (1965) derived the equilibrium equations and the boundary conditions (including the extra ones) for a second strain gradient elasticity theory making use of a stationarity principle (substantially equivalent to the virtual work principle); see also Germain (1973) for a systematic use of the virtual work principle to the same purpose.

In the following, a gradient elasticity theory like the above, being a special polar-type continuum theory, will be referred to as (Toupin–Mindlin) *polar-gradient* elasticity theory. This label aims at distinguishing a polar-gradient theory from other types of polar theories, e.g. the polar-functional theory of Green and Rivlin (1965). It also introduces a net distinction between a polar-gradient theory (of local nature, with gradient characteristics injected at the structural level through the strain–displacement relations) and a true gradient theory as meant in the modern literature (the gradient characteristics are incorporated in the constitutive equations). The latter theory will be referred to simply as *gradient* elasticity theory in the following.

In a gradient elasticity theory, the material strain states can still be considered described by the same set of $n+1$ strain tensors $\boldsymbol{\varepsilon}^{(\nu)}$ of a polar-gradient theory; but—at difference with the latter theory—the n higher order strain tensors are treated, at the constitutive level, as dependent on the strain tensor $\boldsymbol{\varepsilon}^{(0)} = \boldsymbol{\varepsilon}$ through the differential relations (2), or (1). This amounts at introducing, into the material constitutive behavior, an *internal constraint* by which only *displacement-driven strain modes* are allowed, that is, generated by any C^{n+1}-continuous displacement field, $\mathbf{u}$, specified throughout the (Euclidean) domain occupied by the material particle system.

The latter kinematic restriction on the material model has a number of consequences which make the gradient model substantially different from the polar-gradient one and deserve being mentioned in details since the beginning. The following can be stated:

(i) At difference with the polar-gradient theory—where the material stress states are described by $n+1$ stress tensors $\boldsymbol{\sigma}^{(\nu)}$ $(\nu = 0, 1, \ldots, n)$, respectively work-conjugate of as many (independent) strain tensors

$\boldsymbol{\varepsilon}^{(v)}$—in the gradient theory there is a (symmetric, Cauchy) total stress tensor, $\boldsymbol{\sigma}$, which is expressed in terms of the $n+1$ stress tensors $\boldsymbol{\sigma}^{(v)}$ of the polar-gradient model through a differential relation, and which is work-conjugate of the independent strain tensor $\boldsymbol{\varepsilon}^{(0)} = \boldsymbol{\varepsilon}$.

(ii) At difference with the polar-gradient theory—where the stress–strain laws relate algebraically each of the $n+1$ stress tensors $\boldsymbol{\sigma}^{(v)}$ with the $n+1$ associated strain tensors $\boldsymbol{\varepsilon}^{(v)}$—in the gradient theory the total stress tensor $\boldsymbol{\sigma}$ is related to the independent strain tensor $\boldsymbol{\varepsilon}$ through a tensor-valued PDE, say $\boldsymbol{\sigma} = \mathscr{L}(\boldsymbol{\varepsilon})$, of order $2n$.

(iii) At difference with the polar-gradient theory—in which the (algebraic) stress–strain relations are of local type—in the gradient theory the stress–strain relations are nonlocal in nature, since in fact the differential equation $\boldsymbol{\sigma} = \mathscr{L}(\boldsymbol{\varepsilon})$ cannot be integrated uniquely in the relevant domain (evaluation of a displacement-driven strain field, $\boldsymbol{\varepsilon}$, corresponding to a given $\boldsymbol{\sigma}$ field) without taking into account the appropriate boundary conditions. These boundary conditions are *nonstandard* in character, meaning that their role is not that of conveying boundary data into the relevant boundary-value problem, but rather that of suitably completing the differential description of the material constitutive law. Therefore, these nonstandard boundary conditions do not exhibit the form of an alternative (typical of the standard ones), but are cast in a suitably fixed format to enforce some constitutive requirements.

(iv) At difference with the polar-gradient theory—in which (like in any local continuum theory) the strain energy stored in a material element, or particle, is induced by the strain occurred in the same particle—in the gradient theory such strain energy is related to the overall strain field. This fact, consequence of the nonlocal nature of the material constitution, implies that some long distance energy interchanges of diffusive nature occur in the domain and, consequently, that the classical thermodynamics principle of the local action is not valid. In other words, the material particles influence one another not by contact forces and heat diffusion only (as it would be the case if the mentioned principle was valid), but also by long distance energy interchanges.

(v) At difference with the polar-gradient theory—in which (like in any local continuum theory) the first thermodynamics principle holds in its classical pointwise form—in the gradient theory the mentioned principle can be enforced only in global form for the whole domain; but, if enforced in pointwise form for every material element, the aforementioned long distance energy interchanges must be taken in due account, in general through a suitable nonlocality (energy) residual, Edelen and Laws (1971).

Gradient material models emerged in the literature, together with nonlocal integral ones, in the purpose to account for long distance cohesive forces in real structured materials, see e.g. Kröner (1967), Krumhansl (1968), Eringen (1972, 1976, 1987), Rogula (1982), Aifantis (1984a,b, 1999), Triantafyllidis and Aifantis (1986), Altan and Aifantis (1997). Both types of models have recently become popular for their ability in providing remedies to some shortcomings that show up with the classical continuum theories, as for instance the crack-tip stress singularity predicted by classical elasticity, Eringen (1987), and the strain localization predicted by classical plasticity theory in the presence of softening, or damage, Pijaudie-Cabot and Bazant (1987), Aifantis (1984b), Lasry and Belytscko (1988), Mühlhaus and Aifantis (1991), de Borst et al. (1993, 1995). For a review of recent developments in gradient theories see Aifantis (2003) and the references therein.

The concept of nonlocality residual was introduced in the framework of general nonlocal continuum theories, Edelen and Laws (1971), Eringen and Edelen (1972), Eringen (1972), in which a term as nonlocality residual was considered for every balance equation, what made rather cumbersome the resulting theories. Nowadays there is some agreement in considering (like in the present study) just a single nonlocality residual in the internal energy balance equation for every nonlocality source (for instance, elasticity, plasticity and damage). A single nonlocality residual in the form $R = \nabla \cdot \mathbf{w}$ was introduced by Dunn and Serrin (1985), who named the vector $\mathbf{w}$ "interstitial work flux", and by Maugin (1990), who named $\mathbf{w}$ "extra entropy flux", but none of the latter authors took into account the body's constitutive insulation condition (see Section 2). A single nonlocality residual was employed also by Polizzotto (2001) within nonlocal elasticity, by Polizzotto and Borino (1998) within gradient plasticity, by Borino et al. (1999) within nonlocal plasticity, and by Liebe et al. (2001), Benvenuti et al. (2002), Borino et al. (1999) within nonlocal damage mechanics.

An important research issue of continuum mechanics is the correct way to write the nonstandard boundary conditions for a gradient material model. These boundary conditions have not been well assessed in the literature so far. In earlier attempts, they were either written intuitively in an analogy with the standard ones, de Borst and Mühlhaus (1992), Altan and Aifantis (1997), Gurtin (2003), or derived from a variational principle related to a particular boundary-value problem to solve, Mühlhaus and Aifantis (1991), Vardulakis and Aifantis (1991), Comi and Perego (1995), Metrikine and Askes (2002). Only recently have these nonstandard boundary conditions been recognized to possess an essentially constitutive nature and hence to constitute a necessary complement of the constitutive equations formulation problem, to be addressed within an appropriate thermodynamics framework, Polizzotto et al. (1998), Polizzotto and Borino (1998), Liebe et al. (2001).

The present paper is devoted to gradient elasticity and has as main purpose the assessment of the thermodynamic restrictions upon the related constitutive equations with particular attention to the associated (nonstandard) boundary conditions. The same topic for a gradient plasticity model will be treated in a separate paper to follow.

The plan of the paper is as follows. In Section 2, a suitable thermodynamic framework able to account for nonlocality is presented. The classical Clausius–Duhem inequality is modified by the addition of the nonlocality residual and then, in Section 3, used to find the thermodynamic restrictions upon the constitutive equations: it is so found that these equations include, besides the field (differential) stress–strain laws, also a set of (nonstandard) boundary conditions. Also, consistently with these thermodynamic requirements, a surface layer with membrane stresses is envisioned to exist in the strained body. In Section 4, the constitutive expression of the nonlocality residual is determined; moreover, it is proved that, for a gradient material model, the nonlocality residual cannot be identically vanishing. In Section 5, the total strain energy of a strained body is determined and found to include bulk and surface energies. A minimum total potential energy principle for the structural boundary-value problem in gradient elasticity is also formulated. In Section 6, the polar-gradient material model is addressed, comparisons with the gradient model are made and results of Mindlin (1965) are recovered, pointing out the differences between the two models, particularly in the constitutive equations and in the boundary conditions that accompany the displacement equilibrium equations. A particular second gradient material model is presented in Section 7. A few applications to a simple bar in tension are reported in Section 8. Section 9 is devoted to the conclusions. The paper includes two appendices: Appendix A for the notation, and Appendix B where an identity (surface integral transformation formula) of frequent application in the text is provided.

2. Problem position and thermodynamic framework

Let a set of material particles regarded as a continuum occupy a (finite) domain V of the three-dimensional Euclidean space and let this domain, in its undeformed configuration, be referred to a Cartesian orthogonal co-ordinate system, say $\mathbf{x} = (x_1, x_2, x_3)$. In the case of local material behavior, it would be sufficient considering a single typical material element, or particle, in order to establish the relevant stress–strain relations, whereas in the present case of nonlocal material behavior, in which the particles influence one another, the entire particle system must be considered.

Let the material be thermo-elastic with a stress–strain law of the type

$$\boldsymbol{\sigma} = \mathbf{F}(\boldsymbol{\varepsilon}, \nabla\boldsymbol{\varepsilon}, \ldots, \nabla^m\boldsymbol{\varepsilon}, T) \quad \text{in } V, \tag{3}$$

where $\boldsymbol{\sigma}$ is a (symmetric, Cauchy) total stress tensor, $\boldsymbol{\varepsilon}$ the (small) strain tensor and T the absolute temperature. In the common terminology, Eq. (3) defines a gradient material model of *grade m*. Eq. (3) should be completed by a sufficient number of boundary conditions over ∂V in order to guarantee a one-to-one correspondence between the stress and strain fields. The thermodynamic consistency of Eq. (3) and the precise form taken on by the associated boundary conditions must be assessed via a thermodynamic approach similar to that in use in classical constitutive equations theory, except that the material nonlocality features must be accounted for in the present case. This is the object of this section.

Because of the long distance energy interchanges between the material particles with one another in any deformation process, but not between the material particles and the exterior world, the first thermodynamics principle can be written in its classical form only for the entire body, Germain et al. (1983), Lemaitre and Chaboche (1990), that is:

$$\int_V \dot{U}\,\mathrm{d}V = \int_V (\boldsymbol{\sigma} : \dot{\boldsymbol{\varepsilon}} + h - \nabla \cdot \mathbf{q})\,\mathrm{d}V, \tag{4}$$

where $U = U(\boldsymbol{\varepsilon}^{(0)}, \boldsymbol{\varepsilon}^{(1)}, \boldsymbol{\varepsilon}^{(2)}, \eta)$ is the internal energy density, function of the strain tensors $\boldsymbol{\varepsilon}^{(v)}$, $(v = 0, 1, 2)$, and of the entropy η, the strain tensors being specified as in Eq. (2) for $n = 2$ (for simplicity, a second strain gradient model is being considered), that is

$$\boldsymbol{\varepsilon}^{(0)} = \boldsymbol{\varepsilon}, \quad \boldsymbol{\varepsilon}^{(1)} = \nabla\boldsymbol{\varepsilon}, \quad \boldsymbol{\varepsilon}^{(2)} = \nabla^2\boldsymbol{\varepsilon}. \tag{5}$$

Also, h is the heat source, $\mathbf{q}$ is the heat conduction vector.

The first principle of classical thermodynamics is usually stated as in Eq. (4), but enforced for any subdomain (even infinitesimal) $V' \subseteq V$, which makes it possible to derive from it such statements as those related to the mass conservation, momentum and moment of momentum, see e.g. Green and Rivlin (1964). In the presence of nonlocality, Eq. (4) holds only for $V' = V$, hence the first principle cannot be employed for deriving the statements mentioned above (these can, however, be obtained by the virtual work principle, Germain (1973)), but it can still be used to derive the thermodynamic restrictions upon the constitutive equations. This task is achieved hereafter.

As in Edelen and Laws (1971), Polizzotto (2001), Polizzotto and Borino (1998), the balance equation (4) can equivalently be written in a pointwise form as

$$\dot{U} = \boldsymbol{\sigma} : \dot{\boldsymbol{\varepsilon}} + h - \nabla \cdot \mathbf{q} + R, \tag{6}$$

where the additional thermodynamic (scalar) variable, R, is the so-called *nonlocality* (energy) *residual*. R represents the power density transmitted to the generic particle at $\mathbf{x} \in V$ by all other particles in V as a consequence of the nonlocality effects diffusion processes promoted by elastic deformations.

Since the latter processes exhaust within V, the following *insulation condition* must be satisfied:

$$\int_V R\,\mathrm{d}V = 0. \tag{7}$$

In classical thermodynamics of (local) deformable materials, the second principle introduces the internal entropy production, η_{int}, and ultimately states that the inequality

$$\dot{\eta}_{\mathrm{int}} := \dot{\eta} - \left[\frac{h}{T} - \nabla T \cdot \left(\frac{\mathbf{q}}{T}\right)\right] \geqslant 0 \quad \forall \mathbf{x} \in V \tag{8}$$

holds for any possible deformation process of the material, and qualifies as reversible the deformation processes for which Eq. (8) is satisfied as an equality. It is a point of the present thermodynamic framework that inequality (8) holds true also in the case of nonlocal, or gradient, material models. In other words, the second thermodynamics principle holds in its local pointwise form for both local and nonlocal, or gradient, materials.

A simple reasoning to support the latter statement is as follows. Assume that, for a nonlocal, or gradient, material, the second principle is valid in a global form, that is

$$\int_V \dot{\eta}_{\text{int}}\, \mathrm{d}V \geqslant 0 \tag{9}$$

for any possible deformation process. Then, there certainly would exist some deformation processes for which inequality (9) is satisfied as an equality and such processes should be qualified as *reversible at the global level, not at the local one*. Since this is physically meaningless, the assumption is to be rejected. Indeed, reversibility and irreversibility are essentially local material properties. This statement was previously anticipated by Polizzotto (2001) and Polizzotto and Borino (1998), but is here reproposed for completeness. In the following, the second principle is thus enforced in the form of Eq. (8) even in the presence of nonlocality, what is in contrast with other authors, e.g. Edelen and Laws (1971).

Introducing the Helmholtz free energy $\psi = \psi(\boldsymbol{\varepsilon}^{(0)}, \boldsymbol{\varepsilon}^{(1)}, \boldsymbol{\varepsilon}^{(2)}, T)$ by means of the Legendre transformation $\psi = U - T\eta$, Eq. (6) can be rewritten in the following equivalent form:

$$T\dot{\eta}_{\text{int}} = \boldsymbol{\sigma} : \dot{\boldsymbol{\varepsilon}} - \dot{\psi} - \eta\dot{T} - \nabla T \cdot \left(\frac{\mathbf{q}}{T}\right) + R \geqslant 0 \quad \text{in } V, \tag{10}$$

where the inequality sign on the right side is due to Eq. (8). Eq. (10) is the Clausius–Duhem inequality for a nonlocal, or gradient, material; it differs from its classical form only in the presence of the nonlocality residual R. Inequality (10) will be used (in next section) for deriving the desired thermodynamic restrictions upon the constitutive laws of the considered gradient model. Before doing this, it is worth making a few considerations to better clarify the role and the meaning of the nonlocality residual R.

For simplicity of reasoning, isothermal deformation processes are here considered. Then, integration of (10) over V and taking into account Eq. (7) yields

$$\int_V \boldsymbol{\sigma} : \dot{\boldsymbol{\varepsilon}}\, \mathrm{d}V = \int_V \dot{\psi}|_{T=\text{const}}\, \mathrm{d}V + T \int_V \dot{\eta}_{\text{int}}\, \mathrm{d}V. \tag{11}$$

This expresses a classical energy balance relation, that is, the total mechanical work imparted to the system is in part stored as potential energy in the system's microstructure (first integral on the right side), in the remaining part is dissipated as heat (second integral on the right-hand side). But this energy balance is valid only for the whole body, not locally at the generic point where the energy balance relation, by (10), can be written as

$$\boldsymbol{\sigma} : \dot{\boldsymbol{\varepsilon}} + R = \dot{\psi}|_{T=\text{const}} + T\dot{\eta}_{\text{int}}. \tag{12}$$

One can state—at parity of the $\dot{\boldsymbol{\varepsilon}}$ field, hence of $\dot{\psi}$—that, as a consequence of the energy flow due to nonlocality, the total mechanical work (left-hand side of (11)) *redistributes* in V with reductions in the zones where $R > 0$ and increasing in those where $R < 0$, and that thus the nonlocality energy flow proceeds from the latter zones ($R < 0$) to the former ones ($R > 0$). It is thus evident the central role played by R in the energy redistribution processes: namely, at the generic point of V, the mechanical power $\boldsymbol{\sigma} : \dot{\boldsymbol{\varepsilon}}$, augmented by the energy flowing from all other points of the body in the amount R (either positive or negative), splits locally according to the reminded classical rule for the whole body.

3. The gradient elastic model

This section is devoted to the derivation of the thermodynamic restrictions upon the constitutive equations of the gradient material model introduced in Section 2, including the obtainment of the associated boundary conditions. Since a second strain gradient material model is being considered, the

Helmholtz free energy has the form $\psi = \psi(\boldsymbol{\varepsilon}^{(0)}, \boldsymbol{\varepsilon}^{(1)}, \boldsymbol{\varepsilon}^{(2)}, T)$ where, like in (5), $\boldsymbol{\varepsilon}^{(0)} = \{\varepsilon_{ij}\}$ is the usual (symmetric, second-order) strain tensor (six independent components), $\boldsymbol{\varepsilon}^{(1)} = \{\partial_p \varepsilon_{ij}\}$ is a third-order strain tensor, symmetric in the last two index positions (18 independent components) and $\boldsymbol{\varepsilon}^{(2)} = \{\partial_p \partial_q \varepsilon_{ij}\}$ is a fourth-order strain tensor, symmetric in the first two and in the last two index positions (30 independent components). The well-known procedure of Colemann and Gurtin (1967) is used hereafter, see also Germain et al. (1983), Lemaitre and Chaboche (1990).

Integration of (10) over V, expanding the time derivative of $\psi(\cdot)$, and taking into account (5) with $\dot{\boldsymbol{\varepsilon}} \in C^4$ gives:

$$\int_V T\dot{\eta}_{\text{int}}\,\mathrm{d}V = \int_V \left[\boldsymbol{\sigma} : \dot{\boldsymbol{\varepsilon}} - \boldsymbol{\sigma}^{(0)} : \dot{\boldsymbol{\varepsilon}} - \boldsymbol{\sigma}^{(1)} \vdots \nabla\dot{\boldsymbol{\varepsilon}} - \boldsymbol{\sigma}^{(2)} :: \nabla^2 \dot{\boldsymbol{\varepsilon}}\right] \mathrm{d}V - \int_V \left[\left(\frac{\partial\psi}{\partial T} + \eta\right)\dot{T} + \nabla T \cdot \left(\frac{\mathbf{q}}{T}\right)\right] \mathrm{d}V \geqslant 0, \tag{13}$$

where the following positions hold:

$$\boldsymbol{\sigma}^{(0)} := \frac{\partial\psi}{\partial\boldsymbol{\varepsilon}^{(0)}}, \quad \boldsymbol{\sigma}^{(1)} := \frac{\partial\psi}{\partial\boldsymbol{\varepsilon}^{(1)}}, \quad \boldsymbol{\sigma}^{(2)} := \frac{\partial\psi}{\partial\boldsymbol{\varepsilon}^{(2)}}. \tag{14}$$

The latter equations define the tensor-valued (partial) thermodynamic forces associated, respectively, with $\boldsymbol{\varepsilon}^{(0)}$, $\boldsymbol{\varepsilon}^{(1)}$, $\boldsymbol{\varepsilon}^{(2)}$ considered independent of one another. $\boldsymbol{\sigma}^{(0)} = \{\sigma^{(0)}_{ij}\}$ is a Cauchy-like stress tensor, whereas $\boldsymbol{\sigma}^{(1)} = \{\sigma^{(1)}_{pij}\}$ and $\boldsymbol{\sigma}^{(2)} = \{\sigma^{(2)}_{pqij}\}$ are higher order stress tensors (of third- and fourth-order, respectively), sometimes named "double" and "triple" stresses (Mindlin, 1964, 1965). The above stress tensors, which exhibit the same symmetries as the corresponding strain tensors, will be referred to as *microstress tensors* in the following.

Applying the divergence theorem where appropriate, one can write

$$\int_V \boldsymbol{\sigma}^{(1)} \vdots \nabla\dot{\boldsymbol{\varepsilon}}\,\mathrm{d}V = -\int_V \nabla \cdot \boldsymbol{\sigma}^{(1)} : \dot{\boldsymbol{\varepsilon}}\,\mathrm{d}V + \int_S \mathbf{n} \cdot \boldsymbol{\sigma}^{(1)} : \dot{\boldsymbol{\varepsilon}}\,\mathrm{d}S, \tag{15}$$

$$\int_V \boldsymbol{\sigma}^{(2)} :: \nabla^2\dot{\boldsymbol{\varepsilon}}\,\mathrm{d}V = \int_V \nabla^2 : \boldsymbol{\sigma}^{(2)} : \dot{\boldsymbol{\varepsilon}}\,\mathrm{d}V - \int_S \mathbf{n}\nabla : \boldsymbol{\sigma}^{(2)} : \dot{\boldsymbol{\varepsilon}}\,\mathrm{d}S + \int_S \mathbf{n} \cdot \boldsymbol{\sigma}^{(2)} \vdots \nabla\dot{\boldsymbol{\varepsilon}}\,\mathrm{d}S. \tag{16}$$

Using the surface integral transformation formula (B.10) (with $\mathbf{n} \cdot \boldsymbol{\sigma}^{(2)}$ and $\dot{\boldsymbol{\varepsilon}}$ in place of **A** and **B**), the second surface integral of (16) can be transformed as follows:

$$\int_S \mathbf{n} \cdot \boldsymbol{\sigma}^{(2)} \vdots \nabla\dot{\boldsymbol{\varepsilon}}\,\mathrm{d}S = \int_V \mathbf{G} \cdot (\mathbf{n} \cdot \boldsymbol{\sigma}^{(2)}) : \dot{\boldsymbol{\varepsilon}}\,\mathrm{d}S + \int_S \mathbf{nn} : \boldsymbol{\sigma}^{(2)} : \partial_n \dot{\boldsymbol{\varepsilon}}\,\mathrm{d}S. \tag{17}$$

Therefore, substituting (17) into (16), then (15) and (16) into (13), the latter equation becomes

$$\int_V T\dot{\eta}_{\text{int}}\,\mathrm{d}V = \int_V [\boldsymbol{\sigma} - \hat{\boldsymbol{\sigma}}] : \dot{\boldsymbol{\varepsilon}}\,\mathrm{d}V - \int_V \left[\left(\frac{\partial\psi}{\partial T} + \eta\right)\dot{T} + \nabla T \cdot \left(\frac{\mathbf{q}}{T}\right)\right] \mathrm{d}V - \int_S \left[\mathbf{P}^{(1)} : \dot{\boldsymbol{\varepsilon}} + \mathbf{P}^{(2)} : \partial_n \dot{\boldsymbol{\varepsilon}}\right] \mathrm{d}S \geqslant 0, \tag{18}$$

where $\hat{\boldsymbol{\sigma}}$ denotes the total thermodynamic force associated to the independent strain $\dot{\boldsymbol{\varepsilon}}$, defined as

$$\hat{\boldsymbol{\sigma}} := \boldsymbol{\sigma}^{(0)} - \nabla \cdot \boldsymbol{\sigma}^{(1)} + \nabla^2 : \boldsymbol{\sigma}^{(2)} \quad \text{in } V \tag{19}$$

and $\mathbf{P}^{(1)}$ and $\mathbf{P}^{(2)}$ are symmetric second-order tensors given by

$$\mathbf{P}^{(1)} := \mathbf{n} \cdot (\boldsymbol{\sigma}^{(1)} - \nabla \cdot \boldsymbol{\sigma}^{(2)}) + \mathbf{G} \cdot (\mathbf{n} \cdot \boldsymbol{\sigma}^{(2)}), \tag{20a}$$

$$\mathbf{P}^{(2)} := \mathbf{nn} : \boldsymbol{\sigma}^{(2)}. \tag{20b}$$

Inequality (18), consequence of the Clausius–Duhem inequality (10), is not in a form suitable for deriving the desired thermodynamic restrictions on the constitutive equations. This is due to the internal kinematic constraint demanding displacement-driven strain fields in order to guarantee their integrability within the domain V. In other words, for a gradient elastic material model, the field $\dot{\boldsymbol{\varepsilon}}$ is to be treated as being driven by the displacement field $\dot{\mathbf{u}} \in C^5$ through the field compatibility relation, $\dot{\boldsymbol{\varepsilon}} = \nabla^s \dot{\mathbf{u}}$. Therefore, using the latter relation, (18) can be rewritten as

$$\int_V T\dot{\eta}_{\text{int}} \mathrm{d}V = \int_V [\boldsymbol{\sigma} - \hat{\boldsymbol{\sigma}}] : \nabla\dot{\mathbf{u}} \mathrm{d}V - \int_V [\left(\frac{\partial\psi}{\partial T} + \eta\right)\dot{T} + \nabla T \cdot \left(\frac{\mathbf{q}}{T}\right)] \mathrm{d}V \\ - \int_S [\mathbf{P}^{(1)} : \nabla\dot{\mathbf{u}} + \mathbf{P}^{(2)} : \partial_n \nabla\dot{\mathbf{u}}] \mathrm{d}S \geqslant 0, \tag{21}$$

where $\nabla^s \dot{\mathbf{u}}$ has been replaced by $\nabla\dot{\mathbf{u}}$ due to the stated symmetries of the stress tensors.

Applying formula (B.10) one can write

$$\int_S \mathbf{P}^{(1)} : \nabla\dot{\mathbf{u}} \mathrm{d}S = \int_S \mathbf{G} \cdot \mathbf{P}^{(1)} \cdot \dot{\mathbf{u}} \mathrm{d}S + \int_S \mathbf{n} \cdot \mathbf{P}^{(1)} \cdot \partial_n \dot{\mathbf{u}} \mathrm{d}S. \tag{22}$$

Furthermore, note that (Mindlin, 1965)

$$\partial_n(\nabla\dot{\mathbf{u}}) = \nabla(\partial_n\dot{\mathbf{u}}) - \nabla(\mathbf{n}\cdot\nabla)\dot{\mathbf{u}} = \nabla(\partial_n\dot{\mathbf{u}}) - (\nabla\mathbf{n})^{\mathrm{T}} \cdot \nabla\dot{\mathbf{u}} = \nabla(\partial_n\dot{\mathbf{u}}) - (\bar{\nabla}\mathbf{n})^{\mathrm{T}} \cdot \nabla\dot{\mathbf{u}}, \tag{23}$$

where

$$\nabla\mathbf{n} = \bar{\nabla}\mathbf{n} = \{\bar{\nabla}_p n_q\} = \left\{\frac{1}{r_\alpha}\lambda_{\alpha p}\lambda_{\alpha q}\right\} \tag{24}$$

and the $\lambda_{\alpha p}$ ($\alpha = 1, 2$) denote the direction cosines of the curvature lines over the (regular) surface S. Thus, making use of (23) and again applying formula (B.10) (with the appropriate changes), one has:

$$\int_S \mathbf{P}^{(2)} : \partial_n(\nabla\dot{\mathbf{u}}) \mathrm{d}S \\ = \int_S \mathbf{G}\cdot\mathbf{P}^{(2)}\cdot\partial_n\dot{\mathbf{u}} \mathrm{d}S + \int_S \mathbf{n}\cdot\mathbf{P}^{(2)}\cdot\partial_n^2\dot{\mathbf{u}} \mathrm{d}S - \int_S \mathbf{G}\cdot\left[(\bar{\nabla}\mathbf{n})^{\mathrm{T}}\cdot\mathbf{P}^{(2)}\right]\cdot\dot{\mathbf{u}} \mathrm{d}S - \int_S \mathbf{n}\cdot\left[(\bar{\nabla}\mathbf{n})^{\mathrm{T}}\cdot\mathbf{P}^{(2)}\right]\cdot\partial_n\dot{\mathbf{u}} \mathrm{d}S. \tag{25}$$

Therefore, noting that $\mathbf{n} \cdot (\bar{\nabla}\mathbf{n}) = \mathbf{0}$, (hence the last integral of (25) is vanishing), substituting (22) and (25) into (21) and applying the divergence theorem to the volume integral of (21), inequality (21) takes on the form:

$$\int_V T\dot{\eta}_{\text{int}} \mathrm{d}V = -\int_V \nabla\cdot(\boldsymbol{\sigma} - \hat{\boldsymbol{\sigma}})\cdot\dot{\mathbf{u}} \mathrm{d}V - \int_V \left[\left(\frac{\partial\psi}{\partial T} + \eta\right)\dot{T} + \nabla T\cdot\left(\frac{\mathbf{q}}{T}\right)\right] \mathrm{d}V \\ + \int_S \left[\mathbf{n}\cdot(\boldsymbol{\sigma} - \hat{\boldsymbol{\sigma}}) - \mathbf{G}\cdot\left(\mathbf{P}^{(1)} - (\bar{\nabla}\mathbf{n})\cdot\mathbf{P}^{(2)}\right)\right]\cdot\dot{\mathbf{u}} \mathrm{d}S - \int_S [\mathbf{n}\cdot\mathbf{P}^{(1)} + \mathbf{G}\cdot\mathbf{P}^{(2)}]\cdot\partial_n\dot{\mathbf{u}} \mathrm{d}S \\ - \int_S [\mathbf{n}\cdot\mathbf{P}^{(2)}]\cdot\partial_n^2\dot{\mathbf{u}} \mathrm{d}S \geqslant 0. \tag{26}$$

This inequality is suitable for deriving the desired thermodynamic restrictions, since $\dot{\mathbf{u}}$, together with its normal derivatives $\partial_n\dot{\mathbf{u}}$ and $\partial_n^2\dot{\mathbf{u}}$, are free variables in $V \cup S$ and S, respectively. For this purpose, let the class of isothermal elastic deformation processes be considered first, such that $\dot{T} = 0$, $\nabla T = \mathbf{0}$ in any such process. Hence inequality (26) simplifies as follows:

$$\int_V T\dot{\eta}_{\text{int}}\,\mathrm{d}V = -\int_V \nabla\cdot(\boldsymbol{\sigma}-\hat{\boldsymbol{\sigma}}).\dot{\mathbf{u}}\,\mathrm{d}V + \int_S \left[\mathbf{n}\cdot(\boldsymbol{\sigma}-\hat{\boldsymbol{\sigma}}) - \mathbf{G}\cdot(\mathbf{P}^{(1)} - (\bar{\nabla}\mathbf{n})\cdot\mathbf{P}^{(2)})\right]\cdot\dot{\mathbf{u}}\,\mathrm{d}S$$
$$-\int_S [\mathbf{n}\cdot\mathbf{P}^{(1)} + \mathbf{G}\cdot\mathbf{P}^{(2)}]\cdot\partial_n\dot{\mathbf{u}}\,\mathrm{d}S - \int_S [\mathbf{n}\cdot\mathbf{P}^{(2)}]\cdot\partial_n^2\dot{\mathbf{u}}\,\mathrm{d}S \geqslant 0. \tag{27}$$

Considered that inequality (27) must hold true for any displacement-driven isothermal deformation mechanism, it follows as necessary and sufficient conditions, that:

$$\nabla\cdot(\boldsymbol{\sigma}-\hat{\boldsymbol{\sigma}}) = \mathbf{0} \text{ in } V, \quad \mathbf{n}\cdot(\boldsymbol{\sigma}-\hat{\boldsymbol{\sigma}}) - \mathbf{T}^{(0)} = \mathbf{0} \text{ on } S, \tag{28}$$

$$\mathbf{T}^{(1)} := \mathbf{n}\cdot\mathbf{P}^{(1)} + \mathbf{G}\cdot\mathbf{P}^{(2)} = \mathbf{0} \quad \text{on } S, \tag{29a}$$

$$\mathbf{T}^{(2)} := \mathbf{n}\cdot\mathbf{P}^{(2)} = \mathbf{0} \quad \text{on } S, \tag{29b}$$

where $\mathbf{T}^{(0)}$ is defined as

$$\mathbf{T}^{(0)} := \mathbf{G}\cdot(\mathbf{P}^{(1)} - (\bar{\nabla}\mathbf{n})\cdot\mathbf{P}^{(2)}). \tag{30}$$

Eqs. (28) and (29a,b) are the thermodynamic restrictions upon the stress–strain relations for isothermal deformation mechanisms that are driven by the displacement field, as it is required within gradient elasticity. Note that the Cauchy stress $\boldsymbol{\sigma}$ is not uniquely determined by (28), since it in fact can be expressed as

$$\boldsymbol{\sigma} = \hat{\boldsymbol{\sigma}} + \boldsymbol{\rho} \quad \text{in } V, \tag{31}$$

where $\boldsymbol{\rho}$ is an arbitrary stress satisfying

$$\nabla\cdot\boldsymbol{\rho} = \mathbf{0} \quad \text{in } V \quad \mathbf{n}\cdot\boldsymbol{\rho} = \mathbf{T}^{(0)} \text{ on } S. \tag{32}$$

In other words, the Cauchy stress $\boldsymbol{\sigma}$ is allowed to differ from the total thermodymamic force $\hat{\boldsymbol{\sigma}}$ by an arbitrary additive stress $\boldsymbol{\rho}$, but self-equilibrated in V and in equilibrium with the traction $\mathbf{T}^{(0)}$ over the boundary surface S.

However, considered that such a stress redundancy is unmotivated in the present context of (stable) elasticity, $\boldsymbol{\rho}$ can be chosen identically vanishing in V, but different from zero in S, such as to satisfy $(32)_2$. Physically, this choice amounts to conjecturing that the traction $\mathbf{T}^{(0)}$ acting on S is totally resisted by some membrane stresses arising in the boundary surface (surface layer) of the strained body. The membrane shape being known, these membrane stresses can be uniquely determined in terms of $\mathbf{T}^{(0)}$.

Further research efforts would be necessary in order to give a more satisfactory validation to the above conjecture, but this point is not further elaborated here. For the purposes of the present paper, it is sufficient to observe that this conjecture is thermodynamically consistent and coherent with the elastic nature of the material endowed with microstructure. Accordingly, one has to set $\boldsymbol{\sigma} = \hat{\boldsymbol{\sigma}}$ in Eq. (28) and to treat $\mathbf{T}^{(0)}$ as it was identically vanishing in any question concerned with equilibrium. With this proviso, Eqs. (28) and (29a,b), remembering (20a,b) and after a few obvious transformations, can be rewritten as follows:

$$\boldsymbol{\sigma} = \hat{\boldsymbol{\sigma}} := \boldsymbol{\sigma}^{(0)} - \nabla\cdot\boldsymbol{\sigma}^{(1)} + \nabla^2 : \boldsymbol{\sigma}^{(2)} \quad \text{in } V, \tag{33}$$

$$\mathbf{T}^{(1)} := \mathbf{n}\cdot\mathbf{P}^{(1)} - \bar{\nabla}\cdot\mathbf{P}^{(2)} = \mathbf{0} \quad \text{on } S, \tag{34a}$$

$$\mathbf{T}^{(2)} := \mathbf{n}\cdot\mathbf{P}^{(2)} = \mathbf{0} \quad \text{on } S. \tag{34b}$$

The latter equations are the inherent state equations which, at difference with classical continuum theories, include both field and boundary equations. The former, through (14), provides the stress–strain laws for the considered (hyperelastic) gradient model, a set of (generally nonlinear) six PDEs of the fourth-order. Eqs. (34a,b) provide the associated *nonstandard* boundary conditions, which impose that the *nonlocality* *diffusion vectors* $\mathbf{T}^{(1)}[\boldsymbol{\varepsilon}]$ and $\mathbf{T}^{(2)}[\boldsymbol{\varepsilon}]$ vanish identically on the boundary surface S. (Note: $\mathbf{T}^{(1)}$ has the dimension of a force per unit length, $\mathbf{T}^{(2)}$ of a force.)

The vectors $\mathbf{T}^{(v)}[\boldsymbol{\varepsilon}]$ $(v = 0, 1, 2)$, describe the long distance energy flux through S towards the exterior world, but no such energy is allowed to traverse S because of the nonstandard boundary conditions (34a,b), as well as because $\mathbf{T}^{(0)}$ is absorbed by the surface layer as membrane stresses.

As a consequence of (33) and (34a,b), inequality (27) is satisfied as an equality, hence $\dot{\eta}_{\rm int} = 0$ identically, which implies that the considered class of isothermal deformation processes are reversible.

The restrictions enforced by (34a,b), as long with the surface layer resisting the traction $\mathbf{T}^{(0)}$, are a consequence of the kinematic internal constraint imposed by the gradient model to the (local) polar-gradient one. They guarantee that, whatever the deformation process—hence independently of the particular boundary-value problem to which the deformation process may be related—the nonlocality effects do not propagate beyond the body's boundary surface (constitutive insulation).

Coming back to general thermo-elastic deformation processes, the assumption is made that Eqs. (33) and (34a,b) remain valid together with the surface layer and membrane stresses therein. This assumption implies that (26) simplifies as follows:

$$\int_V T\dot{\eta}_{\rm int}\,\mathrm{d}V = -\int_V \left(\frac{\partial\psi}{\partial T} + \eta\right)\dot{T}\,\mathrm{d}V - \int_V \nabla T \cdot \left(\frac{\mathbf{q}}{T}\right).\mathrm{d}V \geqslant 0. \tag{35}$$

This inequality holds for any thermo-elastic deformation process and for any possible heat diffusion law, hence for arbitrary $\dot{T}$ fields in V. It can thus be satisfied if, and only if

$$\eta = -\frac{\partial\psi}{\partial T} \quad \text{in } V, \tag{36}$$

$$\Phi_{\rm T} := -\nabla T \cdot \left(\frac{\mathbf{q}}{T}\right) \geqslant 0 \quad \text{in } V. \tag{37}$$

Eq. (36) is a further state equation specifying the constitutive relation for the entropy η, whereas (37) provides the nonnegative dissipation power by thermal diffusion, $\Phi_{\rm T}$.

4. Evaluation of the nonlocality residual

Since heat conduction is, by assumption, a local-type phenomenon, the evaluation of R can be achieved by considering isothermal deformation processes. For this purpose, let one note that, in virtue of (33) and (34a,b) and of $\mathbf{T}^{(0)}$ being resisted by the membrane stresses in the surface layer, Eq. (27) is satisfied as an equality, hence (as already noted) $\dot{\eta}_{\rm int} = 0$ everywhere in V. From (10), which is also an equality, the nonlocality residual R is determined as

$$R = \dot{\psi}|_{T=\text{const}} - \boldsymbol{\sigma} : \dot{\boldsymbol{\varepsilon}} \quad \text{in } V. \tag{38}$$

This, expanding the time derivative of $\psi(\cdot)$ at constant T and using (14) and (33), gives

$$R = \nabla \cdot \boldsymbol{\sigma}^{(1)} : \dot{\boldsymbol{\varepsilon}} + \boldsymbol{\sigma}^{(1)} \vdots \nabla\dot{\boldsymbol{\varepsilon}} - \nabla^2 : \boldsymbol{\sigma}^{(2)} : \dot{\boldsymbol{\varepsilon}} + \boldsymbol{\sigma}^{(2)} :: \nabla^2\dot{\boldsymbol{\varepsilon}} = \nabla \cdot [(\boldsymbol{\sigma}^{(1)} - \nabla \cdot \boldsymbol{\sigma}^{(2)}) : \dot{\boldsymbol{\varepsilon}} + \boldsymbol{\sigma}^{(2)} \vdots \nabla\dot{\boldsymbol{\varepsilon}}] \quad \text{in } V, \tag{39}$$

which can be regarded as the constitutive expression of R for the considered gradient model.

The reasoning developed in Section 3 to derive (33) and (34a,b) has its central part from Eqs. (13)–(19), (20a), (20b), (21)–(27), where only integral forms of the Clausius–Duhem inequality have been used, hence without the explicit involvement of the residual R. This fact may induce one to conjecture that the nonlocality residual R might be a useless and superfluous ingredient of the theory. But this is not the case, as proved hereafter.

Let V_0 be a (regular) subdomain, $V_0 \subseteq V$. The total nonlocality residual in V_0 can be computed by integration of (39) over V_0 and then applying the divergence theorem, so obtaining

$$\int_{V_0} R\,\mathrm{d}V_0 = \int_{S_0} \mathbf{n}\cdot(\boldsymbol{\sigma}^{(1)} - \nabla\cdot\boldsymbol{\sigma}^{(2)}) : \dot{\boldsymbol{\varepsilon}}\,\mathrm{d}S_0 + \int_{S_0} \mathbf{n}\cdot\boldsymbol{\sigma}^{(2)} \vdots \nabla\dot{\boldsymbol{\varepsilon}}\,\mathrm{d}S_0, \tag{40}$$

where $\mathbf{n}$ is the unit external normal to $S_0 = \partial V_0$. The last surface integral of (40) can be transformed by formula (B.10) (with $\mathbf{n}\cdot\sigma^{(2)}$ and $\dot{\boldsymbol{\varepsilon}}$ in place of $\mathbf{A}$ and $\mathbf{B}$), provided all the surface operators there appearing be computed over S_0. Using the positions in (20a,b) and posing $\dot{\boldsymbol{\varepsilon}} = \nabla^{\mathrm{s}}\dot{\mathbf{u}}$, Eq. (40) is found to take the form

$$\int_{V_0} R\,\mathrm{d}V_0 = \int_{S_0} [\mathbf{P}^{(1)} : \nabla\dot{\mathbf{u}} + \mathbf{P}^{(2)} : \nabla\partial_n\dot{\mathbf{u}})]\,\mathrm{d}S_0. \tag{41}$$

Thus, by Eqs. (22) and (25) written for $S = S_0$, using the positions (29a,b) and (30), gives the notable formula

$$\int_{V_0} R\,\mathrm{d}V_0 = \int_{S_0} [\mathbf{T}^{(0)}\cdot\dot{\mathbf{u}} + \mathbf{T}^{(1)}\cdot\partial_n\dot{\mathbf{u}} + \mathbf{T}^{(2)}\cdot\partial_n^2\dot{\mathbf{u}}]\,\mathrm{d}S_0, \tag{42}$$

which expresses the total nonlocality residual over the subdomain V_0 in terms of the related nonlocality diffusion vectors $\mathbf{T}^{(1)}$ and $\mathbf{T}^{(2)}$, and the traction $\mathbf{T}^{(0)}$ as well, all computed over $S_0 = \partial V_0$.

Indeed, if R was vanishing identically everywhere in V, Eq. (42) would require that

$$\int_{S_0} [\mathbf{T}^{(0)}\cdot\dot{\mathbf{u}} + \mathbf{T}^{(1)}\cdot\partial_n\dot{\mathbf{u}} + \mathbf{T}^{(2)}\cdot\partial_n^2\dot{\mathbf{u}}]\,\mathrm{d}S_0 = 0 \tag{43}$$

for arbitrary choices of $V_0 \subseteq V$ and of the deformation mechanism. This condition can be satisfied if, and only if, $\mathbf{T}^{(0)} = \mathbf{T}^{(1)} = \mathbf{T}^{(2)} = \mathbf{0}$, hence $\boldsymbol{\sigma}^{(1)} = \mathbf{0}$ and $\boldsymbol{\sigma}^{(2)} = \mathbf{0}$, everywhere in V, which implies that the potential $\psi(\cdot)$ does not depend on the strain gradients $\nabla\boldsymbol{\varepsilon}$ and $\nabla^2\boldsymbol{\varepsilon}$ (simple material). Since this is obviously absurd, one can conclude that the nonlocality residual R cannot be identically vanishing for a gradient material. The proof is so acquainted. Gurtin (1965), using different arguments, proved that a strain gradient dependent free energy $\psi(\cdot)$ cannot represent a simple material.

5. Minimum total potential energy principle for gradient elasticity

In the previous sections, a particular gradient thermo-elastic material model has been envisioned. In isothermal conditions—these conditions are assumed throughout in the following—a body of such material obeys the stress–strain laws (14) and (33) with the associated nonstandard boundary conditions (34a,b), and is endowed with a surface layer with membrane stresses equivalent to the traction $\mathbf{T}^{(0)}$, Eq. (30), such that the latter can be treated as identically vanishing in any question regarding equilibrium of the particle system.

In this section, the total strain energy of the body will be assessed first, then a minimum total potential energy principle will be presented.

5.1. Total strain energy

For the gradient particle system, or body, described above, endowed with Helmholtz free energy $\psi(\boldsymbol{\varepsilon}, \nabla\boldsymbol{\varepsilon}, \nabla^2\boldsymbol{\varepsilon})$ and being in a generic strain state $\boldsymbol{\varepsilon}$, let $\dot{\boldsymbol{\varepsilon}}(\mathbf{x}, t') = \nabla^{\mathrm{s}}\dot{\mathbf{u}}(\mathbf{x}, t')$ be the strain rate in any strain path from the initial strain-free state at $t = 0$ to the final strain state $\boldsymbol{\varepsilon}(\mathbf{x}, t) = \nabla^{\mathrm{s}}\mathbf{u}(\mathbf{x}, t)$. The following can be written:

$$\begin{aligned}\int_V \psi(\cdot)\,\mathrm{d}V &= \int_0^t \int_V (\boldsymbol{\sigma}^{(0)} : \dot{\boldsymbol{\varepsilon}} + \boldsymbol{\sigma}^{(1)} \vdots \nabla\dot{\boldsymbol{\varepsilon}} + \boldsymbol{\sigma}^{(2)} :: \nabla^2\dot{\boldsymbol{\varepsilon}})\mathrm{d}V\,\mathrm{d}t' \\ &= \int_V \int_{\mathbf{0}}^{\boldsymbol{\varepsilon}} \boldsymbol{\sigma} : \mathrm{d}\boldsymbol{\varepsilon}\,\mathrm{d}V + \int_0^t \int_S (\mathbf{P}^{(1)} : \dot{\boldsymbol{\varepsilon}} + \mathbf{P}^{(2)} : \partial_n\dot{\boldsymbol{\varepsilon}})\mathrm{d}S\,\mathrm{d}t' \\ &= \int_V \int_{\mathbf{0}}^{\boldsymbol{\varepsilon}} \boldsymbol{\sigma} : \mathrm{d}\boldsymbol{\varepsilon}\,\mathrm{d}V + \int_S \int_{\mathbf{0}}^{\mathbf{u}} \mathbf{T}^{(0)} \cdot \mathrm{d}\mathbf{u}\,\mathrm{d}S + \int_0^t \int_S (\mathbf{T}^{(1)} \cdot \partial_n\dot{\mathbf{u}} + \mathbf{T}^{(2)} \cdot \partial_n^2\dot{\mathbf{u}})\mathrm{d}S\,\mathrm{d}t', \end{aligned} \tag{44}$$

where $\boldsymbol{\sigma}$ is the total stress, Eq. (33).

The integrals

$$W(\boldsymbol{\varepsilon}) := \int_{\mathbf{0}}^{\boldsymbol{\varepsilon}} \boldsymbol{\sigma} : \mathrm{d}\boldsymbol{\varepsilon}, \tag{45a}$$

$$\psi^*(\mathbf{u}) := \int_{\mathbf{0}}^{\mathbf{u}} \mathbf{T}^{(0)} \cdot \mathrm{d}\mathbf{u}, \tag{45b}$$

represent, respectively, the *bulk strain energy density* in V and the *surface strain energy density* in S, which obviously satisfy the following relations:

$$\frac{\partial W}{\partial \boldsymbol{\varepsilon}} = \boldsymbol{\sigma} \quad \frac{\partial \psi^*}{\partial \mathbf{u}} = \mathbf{T}^{(0)}. \tag{46}$$

An initial surface energy value, $\psi_0^* = \psi^*(\mathbf{u} = \mathbf{0})$, may be introduced in (45b) in order to incorporate the surface tension envisioned by Mindlin (1965) in a polar-gradient body, but this point is skipped for simplicity.

Since $\mathbf{T}^{(1)} = \mathbf{T}^{(2)} = \mathbf{0}$ on S by Eqs. (34a,b), Eq. (44) can be rewritten as follows:

$$\int_V \psi(\boldsymbol{\varepsilon}, \nabla\boldsymbol{\varepsilon}, \nabla^2\boldsymbol{\varepsilon})\,\mathrm{d}V = \int_V W(\boldsymbol{\varepsilon})\,\mathrm{d}V + \int_S \psi^*(\mathbf{u})\,\mathrm{d}S. \tag{47}$$

Let one note that the integral on the left-hand side of (47) can be interpreted as the total strain energy in the polar-gradient elastic body being in the strain state $\boldsymbol{\varepsilon}$, whereas the integrals on the right-hand side of (47) are the bulk and surface total strain energies of the gradient elastic body being in the same strain state. This means that the polar-gradient and gradient elastic bodies, having in common the same free energy potential $\psi(\cdot)$ and being in a same strain state, possess equal total strain energies, but *differently distributed* in the respective domains: namely, passing from the polar-gradient body to the gradient one, the total strain energy redistributes, part as bulk strain energy in V, the other part as surface strain energy in the surface layer over S.

5.2. Minimum principle

Let a gradient elastic material as that described previously occupy the domain V of a body subjected to volume forces $\bar{\mathbf{b}}$ in V, tractions $\bar{\mathbf{t}}$ on S_{T} and imposed displacements $\bar{\mathbf{u}}$ on S_{u}, where S_{T} and S_{u} are disjoint complementary portions of the boundary surface S. Imposed thermal-like strains are not considered. In the hypothesis of small displacements and strains, the body's static response to the loads can be found as solution (if it exists) to a boundary-value problem governed by Eqs. (14), (33) and (34a,b)—enriched by the boundary layer with membrane stresses as explained above—, besides the compatibility and equilibrium equations, that is:

$$\boldsymbol{\varepsilon} = \nabla^{\mathrm{s}}\mathbf{u} \ \text{ in } V, \quad \mathbf{u} = \bar{\mathbf{u}} \quad \text{on } S_{\mathrm{u}}, \tag{48a}$$

$$\nabla \cdot \boldsymbol{\sigma} + \mathbf{b} = \mathbf{0} \ \text{ in } V, \quad \mathbf{n} \cdot \boldsymbol{\sigma} = \bar{\mathbf{t}} \ \text{ on } S_T. \tag{48b}$$

The solution to this boundary-value problem is characterized by a minimum principle, as explained hereafter. Let the following functional Π_g be considered, that is:

$$\Pi_g[\mathbf{u}] := \int_V W(\boldsymbol{\varepsilon})\, dV - \int_V \bar{\mathbf{b}} \cdot \mathbf{u}\, dV - \int_{S_T} \bar{\mathbf{t}} \cdot \mathbf{u}\, dS, \tag{49}$$

where $W(\boldsymbol{\varepsilon})$ is the bulk strain energy density, by assumption positive definite, $\boldsymbol{\varepsilon}$ is expressed in terms of $\mathbf{u}$ by $(48a)_1$ and $\mathbf{u} \in C^6$ is the unknown displacement field. The surface strain energy $\psi^*(\mathbf{u})$ does not appear in (49) because $\mathbf{T}^{(0)}$ is conventionally to be treated as vanishing, as previously stated. However, $\psi^*(\mathbf{u})$ can be introduced in (49) by means of (47), so obtaining

$$\Pi_g[\mathbf{u}] = \int_V \psi(\boldsymbol{\varepsilon}, \nabla\boldsymbol{\varepsilon}, \nabla^2\boldsymbol{\varepsilon})\, dV - \int_S \psi^*(\mathbf{u})\, dS - \int_V \bar{\mathbf{b}} \cdot \mathbf{u}\, dV - \int_{S_T} \bar{\mathbf{t}} \cdot \mathbf{u}\, dS. \tag{50}$$

The following can be proven.

Minimum total potential energy principle for gradient elasticity. For a gradient elastic body with a convex free energy potential, the (unique) solution (if exists) to the related boundary-value problem minimizes the total potential energy Π_g (50) of the body under the constraint $\mathbf{u} = \bar{\mathbf{u}}$ on S_u. Conversely, the displacement field $\mathbf{u}$ making minimum Π_g solves the boundary-value problem.

In order to prove the above statement, the first variation of Π_g is considered, that is

$$\delta\Pi_g = \int_V \left[\boldsymbol{\sigma}^{(0)} : \delta\boldsymbol{\varepsilon} + \boldsymbol{\sigma}^{(1)} \vdots \nabla\delta\boldsymbol{\varepsilon} + \boldsymbol{\sigma}^{(2)} :: \nabla^2\delta\boldsymbol{\varepsilon}\right] dV - \int_S \frac{\partial\psi^*}{\partial\mathbf{u}} \cdot \delta\mathbf{u}\, dS - \int_V \bar{\mathbf{b}} \cdot \delta\mathbf{u}\, dV - \int_{S_T} \bar{\mathbf{t}} \cdot \delta\mathbf{u}\, dS, \tag{51}$$

where $\delta\mathbf{u} \in C^6$ is an arbitrary displacement variation, but $\delta\mathbf{u} = \mathbf{0}$ on S_u. Making use of (15)–(17), but with $\dot{\boldsymbol{\varepsilon}}$ replaced by $\delta\boldsymbol{\varepsilon}$, of the definition (19) with $\boldsymbol{\sigma}$ in place of $\hat{\boldsymbol{\sigma}}$, and of (20a,b) as well, one obtains:

$$\begin{aligned}\delta\Pi_g = {} & \int_V \boldsymbol{\sigma} : \nabla\delta\mathbf{u}\, dV - \int_V \mathbf{b} \cdot \delta\bar{\mathbf{u}}\, dV - \int_{S_T} \bar{\mathbf{t}} \cdot \delta\mathbf{u}\, dS - \int_S \frac{\partial\psi^*}{\partial\mathbf{u}} \cdot \delta\mathbf{u}\, dS \\ & + \int_S [\mathbf{P}^{(1)} : \nabla\delta\mathbf{u} + \mathbf{P}^{(2)} : \partial_n(\nabla\delta\mathbf{u})]\, dS.\end{aligned} \tag{52}$$

Further, let Eqs. (22) and (25) (with $\dot{\mathbf{u}}$ replaced by $\delta\mathbf{u}$), be used in order to transform the last surface integral on the right side of (52); also, let the divergence theorem be applied to the first volume integral in (52). Then, in view of $(46)_2$, one obtains:

$$\delta\Pi_g = -\int_V (\nabla \cdot \boldsymbol{\sigma} + \bar{\mathbf{b}}) \cdot \delta\mathbf{u}\, dV + \int_{S_T} (\mathbf{n} \cdot \boldsymbol{\sigma} - \bar{\mathbf{t}}) \cdot \delta\mathbf{u}\, dS + \int_S [\mathbf{T}^{(1)} \cdot \partial_n\delta\mathbf{u} + \mathbf{T}^{(2)} \cdot \partial_n^2\delta\mathbf{u}]\, dS. \tag{53}$$

If $\mathbf{u} \in C^6$ is the/a solution of the gradient elasticity problem, hence (14), (33), (34a,b), and (48a,b) are satisfied, it is $\delta\Pi_g[\mathbf{u}] = 0$ identically and $\Pi_g[\mathbf{u}]$ is stationary; conversely, if $\Pi_g[\mathbf{u}]$ is stationary for some $\mathbf{u} \in C^6$, then (53) must vanish identically, hence $\mathbf{u}$ solves the boundary-value problem. The stationarity of $\Pi_g[\mathbf{u}]$ is thus a characterization of the/a solution (if exists).

On the other hand, denoting $\mathbf{u}' = \mathbf{u} + \delta\mathbf{u}$ a varied displacement field obtained from the solution $\mathbf{u}$ with $\delta\mathbf{u} \in C^6$ arbitrary, but $\delta\mathbf{u} = \mathbf{0}$ on S_u, Π_g can correspondingly be written as

$$\Pi_g[\mathbf{u}'] = \Pi_g[\mathbf{u}] + \delta\Pi_g + \frac{1}{2}\delta^2\Pi_g + O(\|\delta\mathbf{u}\|^3). \tag{54}$$

Because $\delta\Pi_g = 0$ and moreover, for any nontrivial $\delta\boldsymbol{\varepsilon}$ in V,

$$\delta^2\Pi_g = \int_V \delta^2 W(\boldsymbol{\varepsilon})\,\mathrm{d}V > 0 \tag{55}$$

due to the positive definiteness of $W(\boldsymbol{\varepsilon})$, it follows that

$$\Pi_g[\mathbf{u}'] \geqslant \Pi_g[\mathbf{u}] \tag{56}$$

for any $\mathbf{u}'$ belonging to a sufficiently small neighbour functional domain around $\mathbf{u}$, the equality being valid if, and only if, $\mathbf{u}' \equiv \mathbf{u}$ (uniqueness of the solution, if any). The proof is so complete.

6. The polar-gradient model vs. the gradient model

In this section, the Toupin–Mindlin polar-gradient elasticity model, endowed with the same free energy potential $\psi(\cdot)$ of the gradient one, is addressed for comparison purposes. A first basis of comparison is the total strain energies of the polar-gradient and gradient bodies being in a same strain state. This comparison, made in Section 5.1, leads to the conclusion that the two bodies possess the same amount of total strain energy, but the latter is differently distributed in their respective domains, Eq. (47). Further comparisons are elaborated hereafter.

6.1. Thermodynamic aspects

Let $\psi = \psi(\boldsymbol{\varepsilon}^{(0)}, \boldsymbol{\varepsilon}^{(1)}, \boldsymbol{\varepsilon}^{(2)})$ be the common free energy potential. The polar-gradient material is a local-type model with strain and stress states locally described by $\boldsymbol{\varepsilon}^{(v)}$ $(v = 0, 1, 2)$, and $\boldsymbol{\sigma}^{(v)}$ $(v = 0, 1, 2)$, respectively. The Clausius–Duhem inequality (10) holds with $R = 0$ and has the form

$$\boldsymbol{\sigma}^{(0)} : \dot{\boldsymbol{\varepsilon}}^{(0)} + \boldsymbol{\sigma}^{(1)} \vdots \dot{\boldsymbol{\varepsilon}}^{(1)} + \boldsymbol{\sigma}^{(2)} :: \dot{\boldsymbol{\varepsilon}}^{(2)} - \dot{\psi} \geqslant 0 \tag{57}$$

for every individual material particle in V. Expanding the time derivative of ψ, Eq. (57) becomes

$$\left(\boldsymbol{\sigma}^{(0)} - \frac{\partial\psi}{\partial\boldsymbol{\varepsilon}^{(0)}}\right) : \dot{\boldsymbol{\varepsilon}}^{(0)} + \left(\boldsymbol{\sigma}^{(1)} - \frac{\partial\psi}{\partial\boldsymbol{\varepsilon}^{(1)}}\right) \vdots \dot{\boldsymbol{\varepsilon}}^{(1)} + \left(\boldsymbol{\sigma}^{(2)} - \frac{\partial\psi}{\partial\boldsymbol{\varepsilon}^{(2)}}\right) :: \dot{\boldsymbol{\varepsilon}}^{(2)} \geqslant 0. \tag{58}$$

This, since must be satisfied for any deformation mechanism, hence for arbitrary choices of $\dot{\boldsymbol{\varepsilon}}^{(0)}$, $\dot{\boldsymbol{\varepsilon}}^{(1)}$ and $\dot{\boldsymbol{\varepsilon}}^{(2)}$, implies the equalities

$$\boldsymbol{\sigma}^{(0)} = \frac{\partial\psi}{\partial\boldsymbol{\varepsilon}^{(0)}}, \quad \boldsymbol{\sigma}^{(1)} = \frac{\partial\psi}{\partial\boldsymbol{\varepsilon}^{(1)}}, \quad \boldsymbol{\sigma}^{(2)} = \frac{\partial\psi}{\partial\boldsymbol{\varepsilon}^{(2)}}. \tag{59}$$

These are the state equations of the considered material, formally similar to those in (14), where, however, the stress tensors are given as mere definitions. Eq. (59) provides the stress–strain laws of the (hyperelastic) polar-gradient material model.

If the material model is a gradient one, with $\boldsymbol{\varepsilon}^{(0)} = \boldsymbol{\varepsilon}$, $\boldsymbol{\varepsilon}^{(1)} = \nabla\boldsymbol{\varepsilon}$ and $\boldsymbol{\varepsilon}^{(2)} = \nabla^2\boldsymbol{\varepsilon}$, the equalities in (59) cannot any longer be inferred from (58) because the strain rate tensors are not independent of one another. The assessment of the stress state as a function (or a functional) of the strain state cannot be achieved while resting within the framework of a single material element, and anyway it cannot be inferred uniquely from inequality (58) because there is an excess of stress variables. The correct thermodynamic treatment is then that developed in Section 3.

6.2. Boundary-value problem for the polar-gradient model

Let one consider the functional $\Pi_{\mathrm{p}}[\mathbf{u}]$ defined as follows:

$$\Pi_{\mathrm{p}}[\mathbf{u}] := \int_V \psi(\boldsymbol{\varepsilon}^{(0)}, \boldsymbol{\varepsilon}^{(1)}, \boldsymbol{\varepsilon}^{(2)})\,\mathrm{d}V - \int_V \bar{\mathbf{b}} \cdot \mathbf{u}\,\mathrm{d}V - \int_{S_{\mathrm{T}}} \left[\bar{\mathbf{t}} \cdot \mathbf{u} + \bar{\mathbf{t}}^{(1)} \cdot \partial_n \mathbf{u} + \bar{\mathbf{t}}^{(2)} \cdot \partial_n^2 \mathbf{u}\right] \mathrm{d}S, \tag{60}$$

where $\bar{\mathbf{t}}^{(1)}$ and $\bar{\mathbf{t}}^{(2)}$ denote double and triple forces (or generalized tractions) assigned over S_{T} (Mindlin, 1965) and the strain tensors $\boldsymbol{\varepsilon}^{(v)}$ $(v = 0, 1, 2)$, are related to the (unknown) displacement, $\mathbf{u}$, through the field compatibility equations, that is

$$\boldsymbol{\varepsilon}^{(0)} = \nabla^{\mathrm{s}}\mathbf{u}, \quad \boldsymbol{\varepsilon}^{(1)} = \nabla\nabla^{\mathrm{s}}\mathbf{u}, \quad \boldsymbol{\varepsilon}^{(2)} = \nabla^2\nabla^{\mathrm{s}}\mathbf{u} \ \text{ in } V. \tag{61}$$

$\Pi_{\mathrm{p}}[\mathbf{u}]$ is the total potential energy of a polar-gradient body. The first variation of Π_{p}, proceeding in a way similar to that of Section 5.2, can be written as follows:

$$\begin{aligned}\delta\Pi_{\mathrm{p}} = & \int_V \left(\boldsymbol{\sigma}^{(0)} - \nabla \cdot \boldsymbol{\sigma}^{(1)} + \nabla^2 : \boldsymbol{\sigma}^{(2)}\right) : \nabla\delta\mathbf{u}\,\mathrm{d}V \\ & + \int_S \left[\mathbf{P}^{(1)} : \nabla\delta\mathbf{u} + \mathbf{P}^{(2)} : \partial_n(\nabla\delta\mathbf{u})\right]\mathrm{d}S - \int_V \bar{\mathbf{b}} \cdot \delta\mathbf{u}\,\mathrm{d}V \\ & - \int_{S_{\mathrm{T}}} (\bar{\mathbf{t}} \cdot \delta\mathbf{u} + \bar{\mathbf{t}}^{(1)} \cdot \partial_n\delta\mathbf{u} + \bar{\mathbf{t}}^{(2)} \cdot \partial_n^2\delta\mathbf{u})\mathrm{d}S, \end{aligned} \tag{62}$$

where $\nabla^{\mathrm{s}}\mathbf{u}$ has been replaced with $\nabla\mathbf{u}$ for the assumed symmetries in the tensors $\boldsymbol{\sigma}^{(v)}$ $(v = 0, 1, 2)$, and $\mathbf{P}^{(1)}$ and $\mathbf{P}^{(2)}$ are as in (20a,b). Eq. (62), by the divergence theorem, transforms into

$$\begin{aligned}\delta\Pi_{\mathrm{p}} = & -\int_V \left[\nabla \cdot (\boldsymbol{\sigma}^{(0)} - \nabla \cdot \boldsymbol{\sigma}^{(1)} + \nabla^2 : \boldsymbol{\sigma}^{(2)}) + \bar{\mathbf{b}}\right] \cdot \delta\mathbf{u}\,\mathrm{d}V + \int_{S_{\mathrm{T}}} [\mathbf{n} \cdot \left(\boldsymbol{\sigma}^{(0)} - \nabla \cdot \boldsymbol{\sigma}^{(1)} + \nabla^2 : \boldsymbol{\sigma}^{(2)}\right) - \bar{\mathbf{t}}] \cdot \delta\mathbf{u}\,\mathrm{d}S \\ & - \int_{S_{\mathrm{T}}} (\bar{\mathbf{t}}^{(1)} \cdot \partial_n\delta\mathbf{u} + \bar{\mathbf{t}}^{(2)} \cdot \partial_n^2\delta\mathbf{u})\,\mathrm{d}S + \int_S [\mathbf{P}^{(1)} : \nabla\delta\mathbf{u} + \mathbf{P}^{(2)} : \partial_n(\nabla\delta\mathbf{u})]\,\mathrm{d}S. \end{aligned} \tag{63}$$

Further, let Eqs. (22) and (26), with $\dot{\mathbf{u}}$ replaced by $\delta\mathbf{u}$, be applied to transform the last surface integral of (63). In this way, one obtains

$$\begin{aligned}\delta\Pi_{\mathrm{p}} = & -\int_V \left[\nabla \cdot (\sigma^{(0)} - \nabla \cdot \boldsymbol{\sigma}^{(1)} + \nabla^2 : \boldsymbol{\sigma}^{(2)}) + \bar{\mathbf{b}}\right] \cdot \delta\mathbf{u}\,\mathrm{d}V \\ & + \int_{S_{\mathrm{T}}} \left[\mathbf{n} \cdot (\boldsymbol{\sigma}^{(0)} - \nabla \cdot \boldsymbol{\sigma}^{(1)} + \nabla^2 : \boldsymbol{\sigma}^{(2)}) + \mathbf{T}^{(0)} - \bar{\mathbf{t}}\right] \cdot \delta\mathbf{u}\,\mathrm{d}S + \int_S [\mathbf{T}^{(1)} - \bar{\mathbf{t}}^{(1)}] \cdot \partial_n\delta\mathbf{u}\mathrm{d}S \\ & + \int_S [\mathbf{T}^{(2)} - \bar{\mathbf{t}}^{(2)}] \cdot \partial_n^2\delta\mathbf{u}\,\mathrm{d}S. \end{aligned} \tag{64}$$

Let one note that, since no surface layer with membrane stresses exists in the polar-gradient elastic body, the traction $\mathbf{T}^{(0)}$ cannot be disregarded, nor the vectors $\mathbf{T}^{(1)}$ and $\mathbf{T}^{(2)}$ turn out to be required to vanish.

Eq. (64), considering the vectors $\mathbf{T}^{(v)}$ $(v = 0, 1, 2)$, displacement dependent through the side equation $\boldsymbol{\varepsilon} = \nabla^{\mathrm{s}}\mathbf{u}$, represents the first variation of the total potential energy Π_{p} of the polar-gradient body, for which the displacement $\mathbf{u}$ is the driving independent variable field. As it is evident from (64), the Euler–Lagrange equations related to the stationarity for Π_{p} include, besides the compatibility equations, also the field equilibrium equations, i.e.

$$\nabla \cdot (\boldsymbol{\sigma}^{(0)} - \nabla \cdot \boldsymbol{\sigma}^{(1)} + \nabla^2 : \boldsymbol{\sigma}^{(2)}) + \bar{\mathbf{b}} = \mathbf{0} \quad \text{in } V, \tag{65}$$

as well as the related *standard* boundary conditions, that is

- Static boundary conditions on $S_{\rm T}$

$$\mathbf{n}\cdot(\boldsymbol{\sigma}^{(0)}-\nabla\cdot\boldsymbol{\sigma}^{(1)}+\nabla^2:\boldsymbol{\sigma}^{(2)})+\mathbf{T}^{(0)}=\bar{\mathbf{t}}, \tag{66a}$$

$$\mathbf{T}^{(1)}=\bar{\mathbf{t}}^{(1)},\quad \mathbf{T}^{(2)}=\bar{\mathbf{t}}^{(2)}. \tag{66b}$$

- Kinematic boundary conditions on $S_{\rm u}$

$$\mathbf{u}=\bar{\mathbf{u}},\quad \partial_n\mathbf{u}=\bar{\mathbf{u}}^{(1)},\quad \partial_n^2\mathbf{u}=\bar{\mathbf{u}}^{(2)}, \tag{66c}$$

where $\bar{\mathbf{t}}^{(v)}$, $\bar{\mathbf{u}}^{(v)}$ $(v=1,2)$, denote generalized tractions and displacements specified over $S_{\rm T}$ and $S_{\rm u}$. (Different surface partitions, say $S^{(v)}\cup S^{(v)}=S$, for the boundary data can be adopted, but this point has not been pursed for simplicity.) The boundary conditions in (66a–c) coincide with those given by Mindlin (1965).

The solution (if any) to the equation set (59), (61), (65) and (66a–c), which governs the polar-gradient boundary-value problem, is characterized by the stationarity of $\Pi_{\rm p}[\mathbf{u}]$ of (60) under the conditions (61) and (66c), as shown by Mindlin (1965), who also proved that the related solving displacement equation system is the same whether the field compatibility equations are taken as in (61), or even in the form

$$\boldsymbol{\varepsilon}^{(0)}=\nabla^{\rm s}\mathbf{u},\quad \boldsymbol{\varepsilon}^{(1)}=\nabla^2\mathbf{u},\quad \boldsymbol{\varepsilon}^{(2)}=\nabla^3\mathbf{u}\ \text{ in } V. \tag{67}$$

(In relation to the latter point, it is to be noted that the tensors $\nabla\nabla^{\rm s}\mathbf{u}$ and $\nabla^2\mathbf{u}$ possess the same number (eighteen) of independent components and that the components of one tensor are linear combinations of those of the other tensor; the same holds for the tensors $\nabla^2\nabla^{\rm s}$ and $\nabla^3\mathbf{u}$, having thirty independent components each, Mindlin (1965).)

In effects, the previously mentioned stationarity principle can be strengthened by stating the following:

Minimum total potential energy principle for polar-gradient elasticity. For a polar-gradient elastic body with a convex free energy potential, the (unique) solution (if exists) to the related Mindlin-type boundary-value problem minimizes the total potential energy $\Pi_{\rm p}$ of the body under the constraints $\mathbf{u}=\bar{\mathbf{u}}^{(0)}$, $\partial_n\mathbf{u}=\bar{\mathbf{u}}^{(1)}$ and $\partial_n^2\mathbf{u}=\bar{\mathbf{u}}^{(2)}$ on $S_{\rm u}$. Conversely, the variables set that makes minimum the total potential energy $\Pi_{\rm p}$ solves the boundary-value problem.

The proof of the latter statement is easy. Denoting by $\mathbf{u}\in C^6$ the displacement field pertaining to the solution to the boundary-value problem, and by $\delta\mathbf{u}\in C^6$ a displacement variation field such that $\delta\mathbf{u}=\partial_n\delta\mathbf{u}=\partial_n^2\delta\mathbf{u}=\mathbf{0}$ on $S_{\rm u}$, one can write

$$\Pi_{\rm p}[\mathbf{u}']=\Pi_{\rm p}[\mathbf{u}]+\delta\Pi_{\rm p}+\frac{1}{2}\delta^2\Pi_{\rm p}+{\rm O}(\|\delta\mathbf{u}\|^3), \tag{68}$$

where $\mathbf{u}'=\mathbf{u}+\delta\mathbf{u}$. Since $\delta\Pi_{\rm p}=0\ \forall\delta\mathbf{u}$ complying with the side conditions, and since by (60) and the convexity of $\psi(\cdot)$ in the space of its tensor-valued arguments it is

$$\delta^2\Pi_{\rm p}=\int_V\delta^2\psi(\boldsymbol{\varepsilon}^{(0)},\boldsymbol{\varepsilon}^{(1)},\boldsymbol{\varepsilon}^{(2)})\,{\rm d}V>0, \tag{69}$$

follows that

$$\Pi_{\rm p}[\mathbf{u}']\geqslant\Pi_{\rm p}[\mathbf{u}] \tag{70}$$

for any displacement field $\mathbf{u}'$ belonging to a sufficiently small neighbour domain around $\mathbf{u}$, with the equality being valid if, and only if, $\mathbf{u}'\equiv\mathbf{u}$. The proof is so granted.

On comparing the above results with those obtained in Section 5.1, one realizes that the boundary conditions in the two boundary-value problems are *nine* in number for both the gradient and the polar-gradient material models, but whereas in the case of the polar-gradient material all the boundary conditions are standard in nature, in the case of the gradient material there are *three standard* boundary conditions and *six nonstandard* ones.

Another aspect to point out regards the vectors $\mathbf{T}^{(v)}$ $(v = 0, 1, 2)$, which intervene in the above two boundary-value problems, in each with a completely different role. In the polar-gradient problem, these vectors represent some special generalized tractions that arise from the micromorphic nature of the continuum, hence are in general nonvanishing and required to satisfy suitable (static) boundary conditions on S, Eqs. (66a–c). In the gradient problem, the mentioned vectors possess a constitutive nature, $\mathbf{T}^{(1)}$ and $\mathbf{T}^{(2)}$ are the nonlocality diffusion forces and as such are required to vanish identically over the boundary surface (nonstandard boundary conditions), $\mathbf{T}^{(0)}$ promotes the membrane stresses in the surface layer.

7. Particular second gradient material model

As an example, let ψ be taken in the form:

$$\psi := \frac{1}{2}\mathbf{D} :: \boldsymbol{\varepsilon}\boldsymbol{\varepsilon} + \frac{1}{2}c_1\mathbf{D} :: (\nabla\boldsymbol{\varepsilon} \cdot \nabla\boldsymbol{\varepsilon}) + \frac{1}{2}c_2\mathbf{D} :: (\nabla^2\boldsymbol{\varepsilon} : \nabla^2\boldsymbol{\varepsilon}), \tag{71}$$

where $\mathbf{D} = \{D_{ijkh}\}$ denotes the usual fourth-order elastic moduli tensor (with its symmetries) and c_1, c_2 are material constants (with dimensions of second and fourth power of a length, respectively). In indicial notation, ψ is

$$\psi = \frac{1}{2}D_{ijkh}(\varepsilon_{ij}\varepsilon_{kh} + c_1\varepsilon_{ij,p}\varepsilon_{kh,p} + c_2\varepsilon_{ij,pq}\varepsilon_{kh,pq}). \tag{72}$$

By (14), one has

$$\sigma_{ij}^{(0)} = D_{khij}\varepsilon_{kh}, \quad \text{or} \quad \boldsymbol{\sigma}^{(0)} = \mathbf{D} : \boldsymbol{\varepsilon}, \tag{73a}$$

$$\sigma_{pij}^{(1)} = c_1 D_{khij}\varepsilon_{kh,p}, \quad \text{or} \quad \boldsymbol{\sigma}^{(1)} = c_1\nabla(\mathbf{D} : \boldsymbol{\varepsilon}), \tag{73b}$$

$$\sigma_{pqij}^{(2)} = c_2 D_{khij}\varepsilon_{kh,pq}, \quad \text{or} \quad \boldsymbol{\sigma}^{(2)} = c_2\nabla^2(\mathbf{D} : \boldsymbol{\varepsilon}). \tag{73c}$$

Hence, by (33), the total stress is, denoting by $|\nabla|^2 := \nabla \cdot \nabla$ the Laplace operator,

$$\boldsymbol{\sigma} = \mathbf{D} : \left(1 - c_1|\nabla|^2 + c_2|\nabla|^4\right)\boldsymbol{\varepsilon}. \tag{74}$$

By (34a,b), the nonstandard boundary conditions, after a few mathematical transformations, prove to be:

$$\mathbf{T}^{(1)} = \mathbf{nn} : \boldsymbol{\sigma}^{(1)} - (\mathbf{nn}\bar{\nabla})^{\mathrm{T}} \vdots \boldsymbol{\sigma}^{(2)} - (\mathbf{n}\bar{\nabla})^{\mathrm{T}} : (\mathbf{n} \cdot \boldsymbol{\sigma}^{(2)}) - \bar{\nabla} \cdot (\mathbf{nn} : \boldsymbol{\sigma}^{(2)}) = \mathbf{0}, \tag{75a}$$

$$\mathbf{T}^{(2)} = \mathbf{nnn} \vdots \boldsymbol{\sigma}^{(2)} = \mathbf{0}, \tag{75b}$$

where $\boldsymbol{\sigma}^{(1)}$ and $\boldsymbol{\sigma}^{(2)}$ are given by (73b,c).

The Aifantis (second grade) model is a special case of the above one, obtained on setting $c_1 = c \neq 0, c_2 = 0$, by which (74) simplifies as

$$\boldsymbol{\sigma} = \mathbf{D} : (1 - c|\nabla|^2)\boldsymbol{\varepsilon} \tag{76}$$

and the nonstandard boundary conditions (75a,b) reduce to

$$\mathbf{T}^{(1)} = \mathbf{nn} : \boldsymbol{\sigma}^{(1)} = c_1\partial_n\mathbf{t}_n^{(0)} = \mathbf{0}, \quad \mathbf{t}_n^{(0)} := \boldsymbol{\sigma}^{(0)} \cdot \mathbf{n}. \tag{77}$$

8. Applications

A few simple applications to a one-dimensional bar model are reported in this section. The bar has length L, is clamped at the end $x = 0$ and subjected to an imposed displacement $u = \bar{u}$ at the other end, $x = L$. The material is gradient elastic with a stress–strain law as in Eqs. (76) and (77) (Aifantis model), which in the present one-dimensional case take on the form:

$$\sigma = E(\varepsilon - c^2\varepsilon'') \quad \forall x \in (0, L) \tag{78a}$$

$$\varepsilon' = 0 \quad \text{at } x = 0 \text{ and } x = L, \tag{78b}$$

where E is the Young modulus, $(\cdot)' := \mathrm{d}(\cdot)/\mathrm{d}x$ and c^2 is used in place of c to stress the positive definiteness of the related free energy potential $\psi(\cdot)$ given by

$$\psi(\varepsilon, \varepsilon') = \frac{1}{2}E[\varepsilon^2 + c^2(\varepsilon')^2]. \tag{79}$$

Eqs. (78a,b) are the one-dimensional counterparts of (33) and (34a,b) for the case of a first strain gradient model. The surface operator $\mathbf{G}$ of (B.9) being trivially vanishing in the present case, the polar traction $\mathbf{T}^{(0)}$ of (30) is also vanishing, hence no boundary membrane stresses exist in the bar. (It is also to be noted that the gradient elasticity problem to solve is equivalent to a particular polar-gradient elasticity problem for the same bar with (standard) boundary conditions $T^{(1)} = 0$ at both end sections (equivalent to (78b)), besides the same kinematic boundary conditions.)

Two different situations are considered in the following, in one the bar is homogeneous, in the other it is (macroscopically) nonhomogeneous (E piecewise constant).

8.1. Homogeneous bar

The displacement response of the bar to the imposed end displacement can be obtained as the solution to the differential equation

$$(u - c^2u'')'' = 0 \quad \text{in } (0, L) \tag{80}$$

with the standard boundary conditions

$$u(0) = 0, \quad u(L) = \bar{u} \tag{81}$$

as long with the nonstandard ones in Eq. (78b), equivalent to

$$u''(0) = u''(L) = 0. \tag{82}$$

The general solution of (80) is

$$u(x) = A_1x + A_2 + B_1 \sinh\frac{x}{c} + B_2 \cosh\frac{x}{c}, \tag{83}$$

where A_1, A_2, B_1, B_2 are constants to be determined by means of (81) and (82). By (82) one obtains

$$B_2 = 0, \quad B_1 \sinh\frac{L}{c} = 0 \rightarrow B_1 = 0 \tag{84}$$

and by (81) one has

$$u(x) = \bar{u}x/L, \quad \sigma = E\bar{u}/L. \tag{85}$$

It thus follows that the gradient solution coincides with the local-type solution. This is not surprising in consideration of the fact that, in a homogeneous bar, the stress being uniform, also the strain must be uniform for a stable bar. As pointed out by Altan and Aifantis (1997), only the usage of extra boundary conditions in the form (78b) leads to a uniform strain response of the bar. This means that, among different forms of extra boundary conditions that may be used to solve the bar problem, only the conditions in (78b), or (82), are consistent with the gradient model, hence they are to be considered as the very nonstandard boundary conditions.

8.2. Nonhomogeneous bar

Let ξ be a new co-ordinate axis in the bar with origin in the bar middle section, such that $x = \xi + L/2$ $(-L/2 \leqslant \xi \leqslant L/2)$, and let the Young modulus be $E^- = E$ for $\xi < 0$ and $E^+ = \mu E$ for $\xi > 0$. The solution to (80), written separately for the two half portions of the bar, has the form:

$$u^+(\xi) = A_1^+\xi + A_2^+ + B_1^+ \sinh\frac{\xi}{c} + B_2^+ \cosh\frac{\xi}{c} \quad (\xi \geqslant 0), \tag{86a}$$

$$u^-(\xi) = A_1^-\xi + A_2^- + B_1^- \sinh\frac{\xi}{c} + B_2^- \cosh\frac{\xi}{c} \quad (\xi \leqslant 0), \tag{86b}$$

where the A_1, A_2 and B_1, B_2 are constants to evaluate by means of the boundary conditions. The standard boundary conditions are as follows:

$$[u(0)] = [u'(0)] = [u''(0)] = 0, \tag{87}$$

$$[\sigma(0)] = 0, \tag{88}$$

$$u(-L/2) = 0, \quad u(L/2) = \bar{u} \tag{89}$$

(where $[(\cdot)(x)]$ denotes jump of $(\cdot)$ at x), the nonstandard ones being like (82). Conditions (87), which enforce the displacement C^2-continuity at $\xi = 0$, imply that

$$A_2^+ = A_2^- := A_2, \quad B_2^+ = B_2^- := B_2, \tag{90}$$

$$A_1^+ - A_1^- + (B_1^+ - B_1^-)/c = 0, \tag{91}$$

whereas by (88) one obtains

$$A_1^- = \mu A_1^+, \tag{92}$$

then, by (82), $u''(-L/2) = u''(L/2) = 0$, and one has

$$B_1^+ = -B_1^- := B_1, \quad B_2 = -B_1 \tanh\frac{L}{2c}. \tag{93}$$

Finally, the displacement response proves to be as follows:

$$u^+(\xi) = \frac{\bar{u}}{(1+\mu)}\left[2\frac{\xi}{L} + \mu - (1-\mu)\frac{c}{L}\left(\sinh\frac{\xi}{c} - \tanh\frac{L}{2c}\cosh\frac{\xi}{c}\right)\right] \quad (\xi > 0), \tag{94a}$$

$$u^-(\xi) = \frac{\bar{u}}{(1+\mu)}\left[2\mu\frac{\xi}{L} + \mu + (1-\mu)\frac{c}{L}\left(\sinh\frac{\xi}{c} + \tanh\frac{L}{2c}\cosh\frac{\xi}{c}\right)\right] \quad (\xi < 0), \tag{94b}$$

whereas the stress response is

$$\sigma = \frac{2E\bar{u}}{(1+\mu)L}. \tag{95}$$

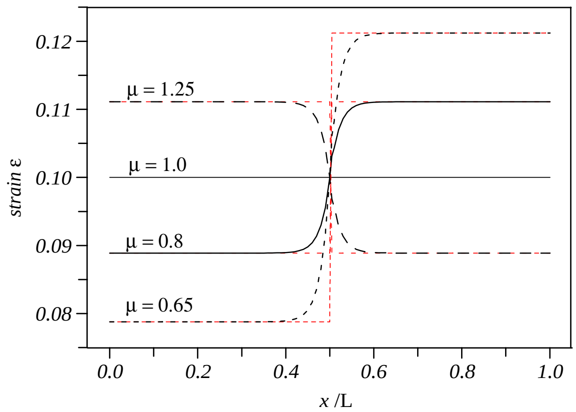

Fig. 1. Strain diagrams in a gradient bar with the Young modulus E in the left half, μE in the right half, subjected to an extension $\bar{u}/L = 0.1$. The discontinuous curves relate to the case of local material.

The strains ε^+ and ε^- as functions of x are given by

$$\varepsilon^+(x) = \frac{\bar{u}}{(1+\mu)L}\left[2 - (1-\mu)\left(\cosh\frac{2x-L}{2c} - \tanh\frac{L}{2c}\sinh\frac{2x-L}{2c}\right)\right] \quad \left(x \geqslant \frac{L}{2}\right), \tag{96a}$$

$$\varepsilon^-(x) = \frac{\bar{u}}{(1+\mu)L}\left[2\mu + (1-\mu)\left(\cosh\frac{2x-L}{2c} + \tanh\frac{L}{2c}\sinh\frac{2x-L}{2c}\right)\right] \quad \left(x \leqslant \frac{L}{2}\right) \tag{96b}$$

and are plotted in Fig. 1.

For $c \to 0$ (local elasticity), the hyperbolic expressions in parentheses of (96a,b) being vanishing at the limit, the strain field proves to be piecewise constant, that is

$$\varepsilon^+ = \frac{2\bar{u}}{(1+\mu)L}, \quad \left(x \geqslant \frac{L}{2}\right); \quad \varepsilon^- = \frac{2\mu\bar{u}}{(1+\mu)L}, \quad \left(x \leqslant \frac{L}{2}\right) \tag{97}$$

as shown in Fig. 1. Also, for $\mu = 1$ the (local type) solution of Section 8.1 is recovered.

9. Conclusions

Gradient elasticity theory, meant as in the modern literature (that is, with the gradient characteristics injected in the constitutive equations), has been discussed mainly from a thermodynamics point of view. Through suitable thermodynamics arguments, the nonstandard boundary conditions for a second gradient model have been provided. Also, in accord with the thermodynamics requirements, a surface layer with membrane stresses has been envisioned in the strained gradient body.

The thermodynamic motivations and the physical meaning of the nonstandard boundary conditions, as well as of the surface layer and membrane stresses therein, have been pointed out. Namely, they guarantee that, in the gradient particle system, the nonlocality effects diffusion processes (causing some energy interchanges within the body) do not exceed the boundary surface of the body, which thus proves to be constitutively insulated.

The essential role played by the nonlocality (energy) residual has been assessed. It makes it possible for the first thermodynamics principle (which for nonlocal continua holds only in global form) to be restated in its classical pointwise form, provided the mentioned nonlocality residual is there involved as an additional state variable. The constitutive expression of the nonlocality residual and the other constitutive equations have been determined through the state equations. The nonlocality residual cannot be identically vanishing for a gradient (or more in general nonlocal) material model, otherwise the material is a simple one.

The total strain energy of a gradient elastic body being in a generic strain state has been shown to include a bulk energy distributed in the domain, and a surface energy distributed in the surface layer. The surface energy may be defined such as to possess an initial value coincident with, or including as a particular case, the surface tension studied by Mindlin (1965).

The structural boundary-value problem for a second gradient hyperelastic body has been addressed in the hypothesis of infinitesimal displacements and a minimum total potential energy principle has been proved. Such a displacement variational formulation is in all aspects similar to the analogous formulation of classical (local) elasticity, except for the presence of two characteristic ingredients, that is, the nonstandard boundary conditions and the surface layer with membrane stresses, which altogether guarantee that no long distance energy flows through the boundary surface towards the exterior.

The polar-gradient elasticity theory studied by Toupin (1962) and Mindlin (1964, 1965) has been also addressed and compared with the herein proposed gradient theory under three points of view, namely: (i) the state equations and related thermodynamic arguments; (ii) the total strain energy of a particle system at a given strain state; (iii) the displacement equilibrium equations and related boundary conditions.

Generalizing the results to a n-th strain gradient material model in a three-dimensional space, the substantial differences between the two models have been pointed out as follows:

(a) The polar-gradient material is local in nature and its strain and stress states are described by two sets of strain and stress tensors as $\boldsymbol{\varepsilon}^{(\nu)}$, $\boldsymbol{\sigma}^{(\nu)}$ $(\nu = 0, 1, \dots, n)$, the latter being work-conjugate of the former, respectively. A gradient material model can be derived from a polar-gradient one by considering the higher order strain tensors $\boldsymbol{\varepsilon}^{(\nu)}$ $(\nu = 1, \dots, n)$, defined as the νth-order spatial gradient of $\boldsymbol{\varepsilon}^{(0)}$, and thus its stress states turn out to be described by a (Cauchy) total stress $\boldsymbol{\sigma}$ work-conjugate of the displacement-driven strain tensor $\boldsymbol{\varepsilon}^{(0)}$.

(b) The stress–strain laws of the polar-gradient model are some algebraic relations of the form $\boldsymbol{\sigma}^{(\nu)} = \boldsymbol{\Phi}_\nu(\boldsymbol{\varepsilon}^{(0)}, \dots, \boldsymbol{\varepsilon}^{(n)})$ $(\nu = 0, 1, \dots, n)$, whereas those of a gradient model are a set of six PDEs of order $2n$ relating $\boldsymbol{\sigma}$ to the displacement-driven strain $\boldsymbol{\varepsilon}$, and include a set of $3n$ nonstandard boundary conditions.

(c) Two equal particle systems of respectively polar-gradient and gradient material, being in a same strain state, possess equal total strain energies, though differently distributed in the volume V for the two models, with bulk and surface energy densities in the gradient one.

(d) For a polar-gradient material body, the solving displacement equilibrium equations have a mathematical structure like in the case of classical local elasticity $(n = 0)$, since in fact they consist in a set of three PDEs of order $2(n + 1)$, accompanied by a set of $3(n + 1)$ (either kinematic, or static) boundary conditions, all of which are standard in nature, that is, they are expressed in the form of an alternative apt to convey (either kinematic, or static) boundary data into the problem. For a gradient material body, the solving displacement equilibrium equations are formally the same as for the polar-gradient body and are accompanied by the same number, $3(n + 1)$, of boundary conditions, three of which are of standard type, the other $3n$ are of nonstandard type.

The present study is being continued for further improvements. In particular, the existence of a surface layer with membrane stresses needs being more satisfactorily justified on the basis of physical and microstructural arguments. Also, solution methods for the structural boundary-value problem need being developed, including FEM analyses, for which the displacement variational formulation here presented would be useful. Here only a few simple applications to a one-dimensional bar in tension have been presented.

Applications of gradient elasticity theory to fracture mechanics problems are of interest (see e.g., Altan and Aifantis, 1997; Vardulakis et al., 1996; Aifantis, 2003), in particular in relation to the crack-tip stress singularity. This has been already proved not to arise within nonlocal (integral) elasticity (Eringen, 1978, 1979), but deserves further study within gradient elasticity. Of interest would be also applications to elasticity problems with the presence of thermal-like strains, whose influence on the gradient material behavior is not a priori obvious. Are the strain gradients entering the gradient law to be gradients of the total strain, or of the elastic one?

The proposed gradient elasticity theory is susceptible of being extended to other gradient material models, as in plasticity and damage mechanics. The extension is by no means a straightforward one. First, because of the way the extended nonstandard boundary conditions must be written: namely, they are to be enforced upon the boundary surface that encloses the subdomain where plasticity, or damage, is being developed and it thus—contrary to the elasticity case—is not coincident, in general, with the external boundary surface, Polizzotto and Borino (1998); second, because the internal kinematic constraint giving rice to the surface layer with membrane stresses proves to be relaxed. This extension will be achieved in a subsequent paper.

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Appendix A. Notation

As a rule, a compact notation is used, with boldface letters to denote vectors and tensors. The scalar product between vectors and tensors is denoted by suitably shaped dot marks, each with as many dots as the number of couples of contracted indices, and each couple being formed with indices having the same location (from the left) in the related tensors. For instance, if $\mathbf{a} = \{a_i\}$, $\mathbf{B} = \{B_{ij}\}$, $\mathbf{C} = \{C_{ijk}\}$ and $\mathbf{D} = \{D_{ijkh}\}$ are a vector and tensors, their scalar products can be written as follows: $\mathbf{a} \cdot \mathbf{B} = \{a_i B_{ij}\}$, $\mathbf{B} : \mathbf{C} = \{B_{ij} D_{ijkh}\}$, $\mathbf{D} \vdots \mathbf{C} = \{D_{ijkh} C_{ijk}\}$, $\mathbf{D} :: (\mathbf{aC}) = \{D_{ijkh} a_i C_{jkh}\}$, where the notation $\mathbf{aC} = \{a_i C_{jkh}\}$ is the tensor product of $\mathbf{a}$ by $\mathbf{C}$ and the index summation rule for repeated indices is applied. Also, e.g., $\mathbf{a} \cdot \mathbf{D} \vdots \mathbf{C} = (\mathbf{a} \cdot \mathbf{D}) \vdots \mathbf{C}$. Orthogonal Cartesian co-ordinates $\mathbf{x} = (x_1, x_2, x_3)$ are used throughout. The symbol $\partial_i(\cdot)$ denotes partial derivative of $(\cdot)$ with respect to x_i, i.e., $\partial_i(\cdot) = \partial(\cdot)/\partial x_i$. The symbol ∇ is the spatial gradient operator, i.e. $\nabla = \{\partial_i\}$, such that $\nabla \mathbf{a} = \{\partial_i a_j\}$, whereas ∇^s is the symmetric part of ∇, i.e. $\nabla^s \mathbf{a} = \{(\partial_i a_j + \partial_j a_i)/2\}$. Also, $\nabla^m = \{\partial_{i_1} \partial_{i_2} \ldots \partial_{i_m}\}$ for any integer $m \geqslant 1$, and the Laplacian operator is indicated as $|\nabla|^2 := \nabla \cdot \nabla = \partial_i \partial_i$. An upper dot indicates time rate, i.e., $\dot{\mathbf{a}} = \partial \mathbf{a}/\partial t$. The symbol $:=$ means equality by definition; also, $(\cdot)^{\mathrm{T}}$ means transpose of $(\cdot)$. Other symbols are defined in the text at their first appearance.

Appendix B. Boundary integral transformation formula

Let $\mathbf{A} = \{A_{pi_1 i_2 \cdots i_m}\}$ and $\mathbf{B} = \{B_{i_1 i_2 \cdots i_m}\}$ be tensors of, respectively, $(m+1)$th- and mth-orders, with $m \geqslant 0$; (for $m = 0$, $\mathbf{A}$ is a vector, $\mathbf{B}$ a scalar). $\mathbf{A}$ is defined over the boundary surface $S = \partial V$ of a spatial domain V, $\mathbf{B}$ over V. Both tensors are by hypothesis sufficiently regular as to make meaningful the surface integral:

$$\int_S \mathbf{A} \odot (\nabla \mathbf{B}) \, \mathrm{d}S = \int_S A_{pi_1 i_2 \cdots i_m} \partial_{\mathrm{p}} B_{i_1 i_2 \cdots i_m} \, \mathrm{d}S. \tag{B.1}$$

The symbol $\odot$ denotes scalar product with complete index contraction for the tensor factor of lower order.

Assuming the surface S regular, let the gradient $\nabla = \{\partial_{\mathrm{p}}\}$ be decomposed in its tangential and normal components at the generic point of S by writing (Mindlin, 1965; Mindlin and Eshel, 1968; Wu, 1992):

$$\nabla = \bar{\nabla} + \mathbf{n}\partial_n \tag{B.2}$$

where denoting by $\mathbf{I} = \{\delta_{ij}\}$ the unit second-order tensor

$$\bar{\nabla} := (\mathbf{I} - \mathbf{nn}) \cdot \nabla, \quad \partial_n := \mathbf{n} \cdot \nabla \tag{B.3}$$

or, in index notation,

$$\bar{\nabla}_p = (\delta_{pq} - n_p n_q)\partial_q, \quad \partial_n = n_q \partial_q. \tag{B.4}$$

Substituting from (B.2) into (B.1) gives

$$\int_S \mathbf{A} \odot (\nabla \mathbf{B})\,\mathrm{d}S = \int_S \mathbf{A} \odot (\bar{\nabla}\mathbf{B})\,\mathrm{d}S + \int_S \mathbf{A} \odot (\mathbf{n}\partial_n \mathbf{B})\,\mathrm{d}S. \tag{B.5}$$

The first integral on the right-hand side of (B.5) can be transformed as follows:

$$\int_S \mathbf{A} \odot (\bar{\nabla}\mathbf{B})\,\mathrm{d}S = \int_S \bar{\nabla} \cdot (\mathbf{A}^{\mathrm{T}} \odot \mathbf{B}^{\mathrm{T}})\,\mathrm{d}S - \int_S (\bar{\nabla} \cdot \mathbf{A}) \odot \mathbf{B}\,\mathrm{d}S. \tag{B.6}$$

By the so-called *surface divergence theorem* (Toupin, 1962; Mindlin, 1965; Wu, 1992), the first integral on the right-hand side of (B.6), in the case of regular surface as assumed here, transforms according to the identity

$$\int_S \bar{\nabla} \cdot (\mathbf{A}^{\mathrm{T}} \odot \mathbf{B}^{\mathrm{T}})\,\mathrm{d}S = \int_S K\mathbf{n} \cdot (\mathbf{A}^{\mathrm{T}} \odot \mathbf{B}^{\mathrm{T}})\,\mathrm{d}S, \tag{B.7}$$

where K equals twice the mean curvature of S at the integration point, that is, denoting by r_1 and r_2 the principal curvature radii,

$$K = \bar{\nabla} \cdot \mathbf{n} = \frac{1}{r_1} + \frac{1}{r_2}. \tag{B.8}$$

Therefore, substituting (B.7) into (B.6), then (B.6) into (B.5), and introducing for more compactness the surface gradient $\mathbf{G} = \{G_\mathrm{p}\}$ defined as

$$\mathbf{G} := K\mathbf{n} - \bar{\nabla}, \tag{B.9}$$

Eq. (B.5) finally takes on the form

$$\int_S \mathbf{A} \odot (\nabla \mathbf{B})\,\mathrm{d}S = \int_S (\mathbf{G} \cdot \mathbf{A}) \odot \mathbf{B}\,\mathrm{d}S + \int_S (\mathbf{n} \cdot \mathbf{A}) \odot \partial_n \mathbf{B}\,\mathrm{d}S. \tag{B.10}$$

The peculiarity of the latter result is that the surface integrals on the right-hand side involve only values of $\mathbf{B}$ and of its normal derivative. The identity (B.10) is of general applicability; it will be referred to as *surface integral transformation formula* in this paper.

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