On constitutive and configurational aspects of models for gradient continua with microstructure*

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Abstract

The purpose of this work is the investigation of some constitutive and configurational aspects of phenomenological model formulations for a class of materials with history-dependent gradient microstructure. The assumption that the behavior of a material point is affected by history-dependent processes in a finite neighbor of this point yields an extended continuum characterized by non-simple material behavior and by additional degrees-of-freedom. This includes both standard micromorphic materials as well as inelastic gradient materials as special cases. As in the case of simple materials, the corresponding constitutive relations are subject to restrictions imposed by material frame-indifference and material symmetry. In the latter case, both direct and differential restrictions are obtained in the case of assuming that the free energy density is an isotropic function of its arguments. In addtion, the concept of material isomorphism is shown to extend to inelastic gradient continua, resulting in a gradient generalization of the well-known elastoplastic multiplicative decomposition of the deformation gradient. Finally, we examine the consequences of gradient extension for the formulation of configurational field and balance relations, and in particular for the Eshelby stress. This is carried out with the help of an incremental stress potential formulation as based on a continuum thermodynamic approach to the coupled field problem involved.

1 Introduction

The behaviour of many materials of engineering interest (*e.g.*, metals, alloys, granular materials, composites, liquid crystals, polycrystals) is often influenced by an existing or emergent microstructure (*e.g.*, phases in multiphase materials, phase transitions, voids, microcracks, dislocation substructures, texture). In general, the components of such a microstructure have different material properties, resulting in a macroscopic material behaviour which is highly anisotropic and inhomogeneous. Attempts to account for these effects in the modeling of such materials have lead to a number of approaches to and viewpoints on the issue depending in particular on the nature of the microstructure in question (*e.g.*, Capriz, 1989; Noll, 1967; Šilhavý, 1997). One class of models idealizing the behavior of such systems phenomenologically is that of gradient continua, including in particular micromorphic materials (*e.g.*, Kafadar and Eringen, 1971; Neff and Forest, 2007) and strain-gradient materials

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(*e.g.*, Fleck and Hutchinson, 1997; Neff *et al.*, 2008) as special cases. As a foundation for the second part of the current work, our first purpose here is to examine some basic constitutive issues for such materials, in particular those of material frame-indifference, material isomorphism and material symmetry. In this, we follow and extend the earlier work of Neff (2008).

Beyond anisotropic and heterogeneous material properties, processes associated with the microstructure which are represented in the model by continuum fields (*e.g.*, damage and order parameter fields, director field) also contribute to configurational fields and processes. Such fields represent additional continuum degrees-of-freedom for which corresponding field relations must be formulated. Contingent on the premise that the corresponding processes contribute to energy flux and energy supply in the material, field relations for such degrees-of-freedom result from the Euclidean frame-indifference of the total rate-of-work (*e.g.*, Capriz, 1989), or more generally from that of the total energy balance (*e.g.*, Capriz and Virga, 1994; Svendsen, 1999, 2001), or even from the exploitation of the dissipation principle (*e.g.*, Levkovitch and Svendsen, 2006). Once thermodynamically-consistent field relations and reduced constitutive relations have been obtained, one is in a position to formulate and solve initial-boundary-value problems. In the context of elastic material behaviour and thermodynamic equilibrium, such initial-boundary-value problems are often formulated variationally. Examples here include elastic phase transitions (*e.g.*, Ball and James, 1987), elastic liquid crystals (*e.g.*, Virga, 1994), configurational fields in elastic materials (*e.g.*, Podio-Guidugli, 2001; Šilhavý, 1997). Formulations for inelastic continua involving configurational fields and balance relations have been examined by a number of workers (*e.g.*, Gurtin, 2002; Menzel and Steinmann, 2000, 2007). Recently, it has been shown (*e.g.*, Carstensen et al., 2003; Miehe, 2002; Ortiz and Repetto, 1999) that direct variational methods for elastic materials can be carried over to the inelastic case with the help of a so-called incremental variational formulation. That this is also the case for the formulation of configurational field and balances has been shown by Svendsen (2005). In the last part of the current work, we apply this approach to the formulation of the Eshelby stress and configurational force balance for the case of gradient materials. For simplicity, the formulation in this work is restricted to isothermal and quasi-static conditions.

Before we begin, a word on notation. Let E^3, V^3, $\mathrm{Lin}(V^3,V^3)$ and $\mathrm{Lin}^+(V^3,V^3)$ represent three-dimensional Euclidean point space, three-dimensional Euclidean vector space, the set of second-order Euclidean tensors, and the set of all such tensors with positive determinant, respectively. Elements of V^3, or mappings taking values in this space, are denoted by bold-face, lower-case $\boldsymbol{a},\ldots$ italic letters. Likewise, upper-case $\boldsymbol{A},\ldots$, italic letters denote elements of $\mathrm{Lin}(V^3,V^3)$, or mappings taking values in this set. In particular, let $\boldsymbol{I}\in\mathrm{Lin}(V^3,V^3)$ represent the second-order identity tensor. The tensor product $\boldsymbol{a}\otimes\boldsymbol{b}$ of any two $\boldsymbol{a},\boldsymbol{b}\in V^3$ is interpreted as an element of $\mathrm{Lin}(V^3,V^3)$ via $(\boldsymbol{a}\otimes\boldsymbol{b})\boldsymbol{c}:=(\boldsymbol{b}\cdot\boldsymbol{c})\boldsymbol{a}$ for all $\boldsymbol{c}\in V^3$. As usual, the inner product on V^3 and trace operation on $\mathrm{Lin}(V^3,V^3)$ induce the scalar product $\boldsymbol{A}\cdot\boldsymbol{B}:=\mathrm{tr}(\boldsymbol{A}^{\mathrm{T}}\boldsymbol{B})$ of any two $\boldsymbol{A},\boldsymbol{B}\in\mathrm{Lin}(V^3,V^3)$. Let $\mathrm{sym}(\boldsymbol{A}):=\frac{1}{2}(\boldsymbol{A}+\boldsymbol{A}^{\mathrm{T}})$, $\mathrm{skw}(\boldsymbol{A}):=\frac{1}{2}(\boldsymbol{A}-\boldsymbol{A}^{\mathrm{T}})$, $\mathrm{sph}(\boldsymbol{A}):=\frac{1}{3}\mathrm{tr}(\boldsymbol{A})\,\boldsymbol{I}$, and $\mathrm{dev}(\boldsymbol{A}):=\boldsymbol{A}-\mathrm{sph}(\boldsymbol{A})$ represent the symmetric, skew-symmetric, spherical, and deviatoric, parts, respectively, of any $\boldsymbol{A}\in\mathrm{Lin}(V^3,V^3)$. Further, let $\mathrm{Sym}(V^3,V^3)$, $\mathrm{Skw}(V^3,V^3)$ and $\mathrm{Orth}(V^3,V^3)$ represent the subsets of $\mathrm{Lin}(V^3,V^3)$ consisting of all symmetric, skew-symmetric, and orthogonal, elements, respectively. Further, let $\mathrm{axi}(\boldsymbol{W})\times\boldsymbol{a}:=\boldsymbol{W}\boldsymbol{a}$ define the axial vector $\mathrm{axi}(\boldsymbol{W})$ of any skew-symmetric tensor $\boldsymbol{W}$, and $\mathrm{axi}(\boldsymbol{w})\boldsymbol{a}:=\boldsymbol{w}\times\boldsymbol{a}$ define the axial tensor of any vector $\boldsymbol{w}$. Third-order Euclidean tensors in this work are interpreted as element of $\mathrm{Lin}(V^3, \mathrm{Lin}(V^3, V^3)) \cong \mathrm{Lin}(\mathrm{Lin}(V^3, V^3), V^3)$. Such tensors, or mappings taking values in these sets, are denoted by upper-case slanted sans-serif characters A, B, and so on. For example, the gradient $\nabla \boldsymbol{T}$ of any second-order tensor field $\boldsymbol{T}$ takes values "naturally" in $\mathrm{Lin}(V^3, \mathrm{Lin}(V^3, V^3))$. In this context, define the switch $(\mathsf{A}^{\mathrm{S}}\boldsymbol{a})\boldsymbol{b} := (\mathsf{A}\boldsymbol{b})\boldsymbol{a}$ of any $\mathsf{A} \in \mathrm{Lin}(V^3, \mathrm{Lin}(V^3, V^3))$ for all $\boldsymbol{a}, \boldsymbol{b} \in V^3$. In turn, this operation induces symmetric $\mathrm{sym}(\mathsf{A}) := \frac{1}{2}(\mathsf{A} + \mathsf{A}^{\mathrm{S}})$, skew-symmetric $\mathrm{skw}(\mathsf{A}) := \frac{1}{2}(\mathsf{A} - \mathsf{A}^{\mathrm{S}})$, and axial $\mathrm{axs}(\mathsf{A}) := \mathrm{axi}(\mathrm{skw}(\mathsf{A}))$, parts of any $\mathsf{A} \in \mathrm{Lin}(V^3, \mathrm{Lin}(V^3, V^3))$. The latter is based on the definition $\mathrm{axi}(\mathsf{W})(\boldsymbol{a} \times \boldsymbol{b}) := 2\,(\mathsf{W}\boldsymbol{a})\boldsymbol{b}$ for all $\boldsymbol{a}, \boldsymbol{b} \in V^3$ of $\mathrm{axi}(\mathsf{W}) \in \mathrm{Lin}(V^3, V^3)$ induced by any $\mathsf{W} \in \mathrm{Lin}(\mathrm{Skw}(V^3, V^3), V^3)$. Finally, we work with the transpose operations $\mathsf{B}^{\mathrm{T}}\mathsf{A} \cdot \boldsymbol{C} := \mathsf{A} \cdot \mathsf{B}\boldsymbol{C}$ and $\mathsf{A}\mathsf{B}^{\mathrm{T}} \cdot \boldsymbol{C} := \mathsf{A} \cdot \boldsymbol{C}\mathsf{B}$ on third-order tensors in this work. Other concepts and definition will be introduced as needed along the way.

2 Basic considerations

The first part of the current work is concerned with material theoretic aspects of model formulations for gradient materials. These include the concepts of material frame-indifference, material isomorphism, material symmetry, and material inhomogeneity. In particular, the latter lies at the basis of the concept of configuration or material forces (*e.g.*, Epstein and Elźanowski, 2007; Gurtin, 2000; Maugin, 1993). Since all of these are intimitely connected with the notion of configuration, or more precisely, placement, of a material body in physical space, *i.e.*, in Euclidean point space E^3, it is useful to express the dependence of the formulation on placement explicitly. To this end, we work with the concept of an abstract material body B (*e.g.*, Noll, 1967). In this setting, any configuration $B_{\boldsymbol{\kappa}} \subset E^3$ of B in E^3 is generated by a corresponding (global) placement $\boldsymbol{\kappa} : B \to E^3$ of B into E^3, *i.e.*, $B_{\boldsymbol{\kappa}} = \boldsymbol{\kappa}[B]$ (*e.g.*, Noll, 1955; Truesdell and Noll, 1992). If $\boldsymbol{\varphi} : B \to Z$ represent a differentiable field on B taking values in some linear or point space Z, let $\nabla^{\boldsymbol{\kappa}}\boldsymbol{\varphi} := \nabla(\boldsymbol{\varphi} \circ \boldsymbol{\kappa}^{-1}) \circ \boldsymbol{\kappa} : B \to \mathrm{Lin}(V^3, Z)$ represents its gradient with respect to $\boldsymbol{\kappa}$. Following Noll (1967), two placements $\boldsymbol{\alpha}, \boldsymbol{\beta} : B \to E^3$ are referred to as being (first-order) equivalent with respect to $\boldsymbol{\kappa}$ at $b \in B$ if $\nabla^{\boldsymbol{\kappa}}\boldsymbol{\alpha}(b) = \nabla^{\boldsymbol{\kappa}}\boldsymbol{\beta}(b)$ holds. Since all members of the class have in this sense the same gradient at b, we follow Noll (1967) and represent the class induced by $\boldsymbol{\kappa}$ at b via the notation $\nabla\boldsymbol{\kappa}(b)$. This equivalence class represents a first-order local placement[1] of $b \in B$ into E^3. Any two such classes $\nabla\boldsymbol{\kappa}(b)$ and $\nabla\boldsymbol{\gamma}(b)$ are related via the transformation relation

$$\nabla\boldsymbol{\gamma}(b) = \nabla^{\boldsymbol{\kappa}}\boldsymbol{\gamma}(b)\nabla\boldsymbol{\kappa}(b)\,. \tag{1}$$

Likewise, the transformation

$$\nabla^{\boldsymbol{\kappa}}\boldsymbol{\varphi}(b) = \nabla^{\boldsymbol{\gamma}}\boldsymbol{\varphi}(b)\nabla^{\boldsymbol{\kappa}}\boldsymbol{\gamma}(b) \tag{2}$$

follows for the gradient at b of any differentiable field $\boldsymbol{\varphi} : B \to Z$ on B with respect to these two classes. Combining these last two relations, one obtains the intrinsic form

$$\nabla\boldsymbol{\varphi}(b) = \nabla^{\boldsymbol{\kappa}}\boldsymbol{\varphi}(b)\nabla\boldsymbol{\kappa}(b) = \nabla^{\boldsymbol{\gamma}}\boldsymbol{\varphi}(b)\nabla\boldsymbol{\gamma}(b) \tag{3}$$

for the gradient of $\boldsymbol{\varphi}$ with respect to the first-order local placements. In the theory of simple materials (*e.g.*, Noll, 1967; Truesdell and Noll, 1992), such first-order local placements and the transformation

[1] In the language of differential geometry, a first-order jet at $b \in B$.

properties of independent constitutive variables such as the deformation gradient with respect to these form the basis for the formulation of concepts such as material isomorphism, uniformity and symmetry. For the current case of (non-simple) gradient materials, however, the notion of local placement must be generalized to higher order (*e.g.*, Cross, 1973; Morgan, 1975; Samohýl, 1981). Two global placements $\boldsymbol{\alpha}, \boldsymbol{\beta}$ are said to be second-order equivalent at $b \in B$ with respect to $\boldsymbol{\kappa}$ (i) if they are first-order equivalent there, and (ii) if $\nabla^{\boldsymbol{\kappa}}\nabla^{\boldsymbol{\kappa}}\boldsymbol{\alpha}(b) = \nabla^{\boldsymbol{\kappa}}\nabla^{\boldsymbol{\kappa}}\boldsymbol{\beta}(b)$ holds. Let $\{\nabla\boldsymbol{\kappa}, \nabla\nabla\boldsymbol{\kappa}\}(b)$ represent the corresponding equivalence class, referred to here as a second-order local placement[2] at $b \in B$. Since these embody the notion of local placement relevant to the formulation of constitutive relations for gradient materials, we refer to them in what follows simply as local placements.

Analogous to (2) in the first-order case, a change of local placement from $\{\nabla\boldsymbol{\kappa}, \nabla\nabla\boldsymbol{\kappa}\}(b)$ to $\{\nabla\boldsymbol{\gamma}, \nabla\nabla\boldsymbol{\gamma}\}(b)$ induces the transformations

$$\begin{aligned} \nabla^{\boldsymbol{\kappa}}\boldsymbol{\varphi}(b) &= \nabla^{\boldsymbol{\gamma}}\boldsymbol{\varphi}(b)\,\nabla^{\boldsymbol{\kappa}}\boldsymbol{\gamma}(b)\,, \\ \nabla^{\boldsymbol{\kappa}}\nabla^{\boldsymbol{\kappa}}\boldsymbol{\varphi}(b) &= \nabla^{\boldsymbol{\gamma}}\nabla^{\boldsymbol{\gamma}}\boldsymbol{\varphi}(b)[\nabla^{\boldsymbol{\kappa}}\boldsymbol{\gamma}(b), \nabla^{\boldsymbol{\kappa}}\boldsymbol{\gamma}(b)] + \nabla^{\boldsymbol{\gamma}}\boldsymbol{\varphi}(b)\,\nabla^{\boldsymbol{\kappa}}\nabla^{\boldsymbol{\kappa}}\boldsymbol{\gamma}(b)\,, \end{aligned} \tag{4}$$

of the first- and second-order gradients at b of any differentiable $\boldsymbol{\varphi}\colon B \rightarrow Z$ with respect to the two classes. Here, $\mathsf{A}[\boldsymbol{B}, \boldsymbol{B}]$ represents the third-order tensor defined by $(\mathsf{A}[\boldsymbol{B}, \boldsymbol{B}]\boldsymbol{a})\boldsymbol{b} := (\mathsf{A}(\boldsymbol{B}\boldsymbol{a}))\boldsymbol{B}\boldsymbol{b}$ for all $\boldsymbol{a}, \boldsymbol{b} \in V^3$. Whereas $(4)_1$ represents a tensor transformation, note that the second term in $(4)_2$ renders this transformation non-tensorial in general. On the other hand, the pair $\{\nabla^{\boldsymbol{\kappa}}\boldsymbol{\varphi}, \nabla^{\boldsymbol{\kappa}}\nabla^{\boldsymbol{\kappa}}\boldsymbol{\varphi}\}(b)$ does transform tensorially[3], *i.e.*,

$$\{\nabla^{\boldsymbol{\kappa}}\boldsymbol{\varphi}, \nabla^{\boldsymbol{\kappa}}\nabla^{\boldsymbol{\kappa}}\boldsymbol{\varphi}\}(b) = \{\nabla^{\boldsymbol{\gamma}}\boldsymbol{\varphi}, \nabla^{\boldsymbol{\gamma}}\nabla^{\boldsymbol{\gamma}}\boldsymbol{\varphi}\}(b) * \{\nabla^{\boldsymbol{\kappa}}\boldsymbol{\gamma}, \nabla^{\boldsymbol{\kappa}}\nabla^{\boldsymbol{\kappa}}\boldsymbol{\gamma}\}(b) \tag{5}$$

via the (second-order) "jet" product

$$\{\boldsymbol{A}, \mathsf{A}\} * \{\boldsymbol{B}, \mathsf{B}\} := \{\boldsymbol{A}\boldsymbol{B}, \mathsf{A}[\boldsymbol{B}, \boldsymbol{B}] + \boldsymbol{A}\mathsf{B}\} \tag{6}$$

on pairs $\{\boldsymbol{A}, \mathsf{A}\}$ and $\{\boldsymbol{B}, \mathsf{B}\}$ of second- and third-order tensors induced by the chain rule for first- and second-order gradients of point- or linear-space-valued fields. From the constitutive point of view, then, (5) is relevant for our purposes here. Analogous to (3) in the first-order case, (4) can be expressed in the intrinsic form

$$\{\nabla\boldsymbol{\varphi}, \nabla\nabla\boldsymbol{\varphi}\}(b) = \{\nabla^{\boldsymbol{\kappa}}\boldsymbol{\varphi}, \nabla^{\boldsymbol{\kappa}}\nabla^{\boldsymbol{\kappa}}\boldsymbol{\varphi}\}(b) * \{\nabla\boldsymbol{\kappa}, \nabla\nabla\boldsymbol{\kappa}\}(b) \tag{7}$$

via (5) and (6). In particular, this holds for the case that $\boldsymbol{\varphi}$ represents a second local placement, *i.e.*, $\boldsymbol{\varphi} \equiv \boldsymbol{\gamma}$.

Using the notion of placement, a motion, or time-dependent deformation, of the body can be represented in abstract form as a continuous sequence of such placements in some time-interval $I \subset$

[2] A second-order jet at $b \in B$. If we were dead set on abstract elegance and generality in the spirit of, for example, Noll (1967), Betounes (1986), or Segev (1994), this would be the point to roll out the full armada of concepts and tools offered by modern differential geometry (*e.g.*, Abraham *et al.*, 1988) such as differential forms. Since the formulation is undoubtedly already sufficiently "scary," however, we refrain from doing this.

[3] This represents a major insight of modern differential geometry which has been exploited for constitutive purposes in, *e.g.*, Cross (1973), Morgan (1975), Samohýl (1981), or Epstein and Elźanowski (2007).

$\mathbb{R}$, *i.e.*, $\boldsymbol{\chi} : I \times B \to E^3$, with $\boldsymbol{\chi}_t := \boldsymbol{\chi}(t, \cdot) \colon B \to B_t$ the placement of B into its current (*i.e.*, time t) configuration $B_t := \boldsymbol{\chi}_t[B]$ in E^3. We have

$$\{\nabla\boldsymbol{\chi}, \nabla\nabla\boldsymbol{\chi}\}(t, b) = \{\nabla^{\boldsymbol{\kappa}}\boldsymbol{\chi}, \nabla^{\boldsymbol{\kappa}}\nabla^{\boldsymbol{\kappa}}\boldsymbol{\chi}\}(t, b) * \{\nabla\boldsymbol{\kappa}, \nabla\nabla\boldsymbol{\kappa}\}(b) \tag{8}$$

from (7) for the representation of the first and second gradients of $\boldsymbol{\chi}$ with respect to $\{\nabla\boldsymbol{\kappa}, \nabla\nabla\boldsymbol{\kappa}\}(b)$ via direct generalization. In the context of simple materials, the history of deformation processes in an infinitesimal neighborhood of $b \in B$, *i.e.*, the history of the deformation gradient $\boldsymbol{F} := \nabla\boldsymbol{\chi}$ at this point, determines its behavior. In particular, we assume that the evolution of the material microstructure influences this local deformation history. For example, in the case of a defect-based microstructure in metallic single or polycrystals, this microstructure consists of vacancies, interstitials, and dislocations. As a model for the (local) deformation of the material microstructure at b at $t \in I$, we work with the local deformation or deformation-gradient-like quantity $\boldsymbol{F}_{\mathrm{M}}(t, b) \in \mathrm{Lin}^+(V^3, V^3)$. Assuming it represents an elastic material isomorphism and induces a stress-free intermediate (local) configuration, for example, $\boldsymbol{F}_{\mathrm{M}}$ can be associated with the "usual" inelastic (local) deformation $\boldsymbol{F}_{\mathrm{P}}$. Or it could represent the microstructural deformation in the context of micromorphic continua (*e.g.*, Kafadar and Eringen, 1971; Neff and Forest, 2007). Besides $\boldsymbol{F}_{\mathrm{M}}(t, b)$ itself, the behavior of any $b \in B$ at a given $t \in I$ is assumed to be influenced by its spatial variation in an infinitesimal spatial neighborhood of b, represented here via the gradient $\nabla\boldsymbol{F}_{\mathrm{M}}(t, b)$ of $\boldsymbol{F}_{\mathrm{M}}(t, b)$ at $(t, b) \in I \times B$. Being a local deformation kinematically analogous to $\boldsymbol{F}$ by definition, it is reasonable to assume that $\boldsymbol{F}_{\mathrm{M}}$ and its gradient have the representation

$$\{\boldsymbol{F}_{\mathrm{M}}, \nabla\boldsymbol{F}_{\mathrm{M}}\}(t, b) = \{\boldsymbol{F}_{\mathrm{M}\boldsymbol{\kappa}}, \nabla^{\boldsymbol{\kappa}}\boldsymbol{F}_{\mathrm{M}\boldsymbol{\kappa}}\}(t, b) * \{\nabla\boldsymbol{\kappa}, \nabla\nabla\boldsymbol{\kappa}\}(b) \tag{9}$$

at b relative to any $\{\nabla\boldsymbol{\kappa}, \nabla\nabla\boldsymbol{\kappa}\}(b)$ formally analogous to (8). In contrast to standard "local" internal variable formulations, note that $\boldsymbol{F}_{\mathrm{M}}$ represents an additional tensor-valued *field* in the formulation at this point, *i.e.*, formally analogous to $\boldsymbol{\chi}$. As such, its constitutive nature is characterized in the current formulation via an *evolution-field* constitutive relation. More on this to follow.

In the current work, the behavior of any material point $b \in B$ is assumed to be influenced in particular by the process of energy storage in a neighborhood $N_b \subset B$ of this point in the material. Conceptually, this can be associated here with the notion of the interaction of the material at $b \in B$ with the surrounding material in the body. In the current case of isothermal inelastic gradient continua, this process is represented by the extended form

$$\psi_b(\mathcal{F}, \mathcal{F}_{\mathrm{M}}) = \psi_{\mathcal{P}_{\boldsymbol{\kappa}}(b)}(\mathcal{F}_{\boldsymbol{\kappa}}, \mathcal{F}_{\mathrm{M}\boldsymbol{\kappa}}) = \psi_{\boldsymbol{\kappa}(b)}(\boldsymbol{F}_{\boldsymbol{\kappa}}, \nabla^{\boldsymbol{\kappa}}\boldsymbol{F}_{\boldsymbol{\kappa}}, \boldsymbol{F}_{\mathrm{M}\boldsymbol{\kappa}}, \nabla^{\boldsymbol{\kappa}}\boldsymbol{F}_{\mathrm{M}\boldsymbol{\kappa}}) \tag{10}$$

for the referential free energy density of the material point $b \in B$ relative to the local placement

$$\mathcal{P}_{\boldsymbol{\kappa}}(b) := \{\nabla\boldsymbol{\kappa}, \nabla\nabla\boldsymbol{\kappa}\}(b) \tag{11}$$

via the definitions

$$\begin{aligned} \mathcal{F}_{\boldsymbol{\kappa}} &:= \{\boldsymbol{F}_{\boldsymbol{\kappa}}, \nabla^{\boldsymbol{\kappa}}\boldsymbol{F}_{\boldsymbol{\kappa}}\} , \\ \mathcal{F}_{\mathrm{M}\boldsymbol{\kappa}} &:= \{\boldsymbol{F}_{\mathrm{M}\boldsymbol{\kappa}}, \nabla^{\boldsymbol{\kappa}}\boldsymbol{F}_{\mathrm{M}\boldsymbol{\kappa}}\} . \end{aligned} \tag{12}$$

Note that this form is tensorial with respect to change of local placement. Indeed, in terms of the notation

$$\mathcal{H}_{\gamma\boldsymbol{\kappa}}(b) := \{\nabla^{\boldsymbol{\kappa}}\gamma, \nabla^{\boldsymbol{\kappa}}\nabla^{\boldsymbol{\kappa}}\gamma\}(b) , \tag{13}$$

one obtains

$$\mathcal{H}_{\boldsymbol{\gamma\kappa}*}(b)\psi_{\mathcal{P}_{\boldsymbol{\kappa}}(b)} = \det(\nabla^{\boldsymbol{\kappa}}\boldsymbol{\gamma}(b))\,\psi_{\mathcal{P}_{\boldsymbol{\gamma}}(b)}\ , \tag{14}$$

for this transformation from $\mathcal{P}_{\boldsymbol{\kappa}}(b)$ to $\mathcal{P}_{\boldsymbol{\gamma}}(b) = \{\nabla\boldsymbol{\gamma}, \nabla\nabla\boldsymbol{\gamma}\}(b)$, *i.e.*,

$$\begin{aligned}\psi_{\mathcal{P}_{\boldsymbol{\kappa}}(b)}(\mathcal{F}_{\boldsymbol{\kappa}}, \mathcal{F}_{\mathrm{M}\boldsymbol{\kappa}}) &= \psi_{\mathcal{P}_{\boldsymbol{\kappa}}(b)}(\mathcal{F}_{\boldsymbol{\gamma}} * \mathcal{H}_{\boldsymbol{\gamma\kappa}}, \mathcal{F}_{\mathrm{M}\boldsymbol{\gamma}} * \mathcal{H}_{\boldsymbol{\gamma\kappa}}) \\ &=: (\mathcal{H}_{\boldsymbol{\gamma\kappa}*}(b)\psi_{\mathcal{P}_{\boldsymbol{\kappa}}(b)})(\mathcal{F}_{\boldsymbol{\gamma}}, \mathcal{F}_{\mathrm{M}\boldsymbol{\gamma}}) \\ &= \det(\nabla^{\boldsymbol{\kappa}}\boldsymbol{\gamma}(b))\,\psi_{\mathcal{P}_{\boldsymbol{\gamma}}(b)}(\mathcal{F}_{\boldsymbol{\gamma}}, \mathcal{F}_{\mathrm{M}\boldsymbol{\gamma}})\ .\end{aligned} \tag{15}$$

In particular, this tensorial character is required for the formulation of material symmetry (*e.g.*, Cross, 1973; Samohýl, 1981; Šilhavý, 1997), an issue which we examine in what follows.

3 Material frame-indifference

Consider next the formulation of restrictions imposed by material frame-indifference on the basic constitutive relation (10) for energy storage in a second-order inelastic gradient material point b. As usual, material frame-indifference is considered in the context of the action of the (representation of the) orthogonal group $\mathrm{Orth}(V^3, V^3)$ with respect to V^3. As discussed for example in detail by Svendsen and Bertram (1999), material frame-indifference is equivalent to requiring Euclidean frame-indifference and form invariance. The formulation of the consequences of this in the current setting is based on the spatial action

$$\begin{aligned}s_{\boldsymbol{Q}}\psi_{\mathcal{P}_{\boldsymbol{\kappa}}(b)}(\mathcal{F}_{\boldsymbol{\kappa}}, \mathcal{F}_{\mathrm{M}\boldsymbol{\kappa}}) &= \psi_{\mathcal{P}_{\boldsymbol{\kappa}}(b)}(s_{\boldsymbol{Q}}\mathcal{F}_{\boldsymbol{\kappa}}, s_{\boldsymbol{Q}}\mathcal{F}_{\mathrm{M}\boldsymbol{\kappa}})\ , \\ &= \psi_{\boldsymbol{\kappa}(b)}(\boldsymbol{Q}\boldsymbol{F}_{\boldsymbol{\kappa}}, \boldsymbol{Q}\nabla^{\boldsymbol{\kappa}}\boldsymbol{F}_{\boldsymbol{\kappa}}, \boldsymbol{F}_{\mathrm{M}\boldsymbol{\kappa}}, \nabla^{\boldsymbol{\kappa}}\boldsymbol{F}_{\mathrm{M}\boldsymbol{\kappa}})\end{aligned} \tag{16}$$

of any element $\boldsymbol{Q} \in \mathrm{Orth}(V^3, V^3)$ of $\mathrm{Orth}(V^3, V^3)$ on the form (10) of the free energy density. In this context, material frame-indifference requires that

$$s_{\boldsymbol{Q}}\psi_{\mathcal{P}_{\boldsymbol{\kappa}}(b)} = \psi_{\mathcal{P}_{\boldsymbol{\kappa}}(b)}\ , \tag{17}$$

i.e.,

$$\psi_{\boldsymbol{\kappa}(b)}(\boldsymbol{F}_{\boldsymbol{\kappa}}, \nabla^{\boldsymbol{\kappa}}\boldsymbol{F}_{\boldsymbol{\kappa}}, \boldsymbol{F}_{\mathrm{M}\boldsymbol{\kappa}}, \nabla^{\boldsymbol{\kappa}}\boldsymbol{F}_{\mathrm{M}\boldsymbol{\kappa}}) = \psi_{\boldsymbol{\kappa}(b)}(\boldsymbol{Q}\boldsymbol{F}_{\boldsymbol{\kappa}}, \boldsymbol{Q}\nabla^{\boldsymbol{\kappa}}\boldsymbol{F}_{\boldsymbol{\kappa}}, \boldsymbol{F}_{\mathrm{M}\boldsymbol{\kappa}}, \nabla^{\boldsymbol{\kappa}}\boldsymbol{F}_{\mathrm{M}\boldsymbol{\kappa}}) \tag{18}$$

for all $\boldsymbol{Q} \in \mathrm{Orth}(V^3, V^3)$. The most common restriction derived from this is of course form reduction (*e.g.*, Bertram and Svendsen, 2001; Šilhavý, 1997; Truesdell and Noll, 1992). As in the case of simple materials, reduction here is based on the arbitraryness of $\psi_{\boldsymbol{\kappa}(b)}$ and $\boldsymbol{Q}$, the latter facilitating the choice $\boldsymbol{Q}(t) \equiv \boldsymbol{R}^{\mathrm{T}}_{\boldsymbol{\kappa}}(t, b)$ in the context of the right polar decomposition $\boldsymbol{F}_{\boldsymbol{\kappa}} = \boldsymbol{R}_{\boldsymbol{\kappa}}\boldsymbol{U}_{\boldsymbol{\kappa}}$. On this basis, there exists a reduced form $\psi_{\mathrm{r}\,\boldsymbol{\kappa}(b)}$ of $\psi_{\boldsymbol{\kappa}(b)}$ such that

$$\psi_{\boldsymbol{\kappa}(b)}(\boldsymbol{F}_{\boldsymbol{\kappa}}, \nabla^{\boldsymbol{\kappa}}\boldsymbol{F}_{\boldsymbol{\kappa}}, \boldsymbol{F}_{\mathrm{M}\boldsymbol{\kappa}}, \nabla^{\boldsymbol{\kappa}}\boldsymbol{F}_{\mathrm{M}\boldsymbol{\kappa}}) = \psi_{\mathrm{r}\,\boldsymbol{\kappa}(b)}(\boldsymbol{C}_{\boldsymbol{\kappa}}, \nabla^{\boldsymbol{\kappa}}\boldsymbol{C}_{\boldsymbol{\kappa}}, \boldsymbol{F}_{\mathrm{M}\boldsymbol{\kappa}}, \nabla^{\boldsymbol{\kappa}}\boldsymbol{F}_{\mathrm{M}\boldsymbol{\kappa}}) \tag{19}$$

holds. In particular, this results follows from the functional relations

$$\begin{aligned}\boldsymbol{C}_{\boldsymbol{\kappa}} &= \boldsymbol{F}^{\mathrm{T}}_{\boldsymbol{\kappa}}\boldsymbol{F}_{\boldsymbol{\kappa}} &&= \boldsymbol{U}_{\boldsymbol{\kappa}}\boldsymbol{U}_{\boldsymbol{\kappa}}\ , \\ \nabla^{\boldsymbol{\kappa}}\boldsymbol{C}_{\boldsymbol{\kappa}} &= (\nabla^{\boldsymbol{\kappa}}\boldsymbol{F}^{\mathrm{T}}_{\boldsymbol{\kappa}})^{\mathrm{S}}\boldsymbol{F}_{\boldsymbol{\kappa}} + \boldsymbol{F}^{\mathrm{T}}_{\boldsymbol{\kappa}}\,\nabla^{\boldsymbol{\kappa}}\boldsymbol{F}_{\boldsymbol{\kappa}} &&= (\nabla^{\boldsymbol{\kappa}}\boldsymbol{U}_{\boldsymbol{\kappa}})^{\mathrm{S}}\boldsymbol{U}_{\boldsymbol{\kappa}} + \boldsymbol{U}_{\boldsymbol{\kappa}}\,\nabla^{\boldsymbol{\kappa}}\boldsymbol{U}_{\boldsymbol{\kappa}}\ ,\end{aligned}$$

between $\boldsymbol{U}_{\boldsymbol{\kappa}}, \boldsymbol{C}_{\boldsymbol{\kappa}}$, and their gradients.

Equally important as the direct restrictions (18) in the context of material frame-indifference are the differential restrictions derived from them (*e.g.*, Šilhavý, 1997, Chapter 8). From a mathematical point of view, these represent retrictions with respect to the Lie algebra $\mathrm{Skw}(V^3, V^3)$ corresponding to the Lie group $\mathrm{Orth}(V^3, V^3)$. To obtain these in the current context, note again that (18) holds for all orthogonal transformations by design. Consequently, it holds in particular with respect to any curve $\boldsymbol{Q}(s) = \exp(\boldsymbol{\Omega}\, s)$ in $\mathrm{Orth}(V^3, V^3)$ generated by the skew-symmetric tensor $\boldsymbol{\Omega} \in \mathrm{Skw}(V^3, V^3)$. Substituting this form for $\boldsymbol{Q}$ into this last result, taking the derivative of the result with respect to s, and setting $s = 0$, one obtains

$$
\begin{aligned}
0 &= \partial_{\boldsymbol{Q}(0)} \psi_{\mathcal{P}_{\boldsymbol{\kappa}}(b)} \cdot \boldsymbol{Q}'(0) \\
&= \partial_{\mathcal{F}_{\boldsymbol{\kappa}}} \psi_{\mathcal{P}_{\boldsymbol{\kappa}}(b)} \cdot s_{\boldsymbol{\Omega}} \mathcal{F}_{\boldsymbol{\kappa}} \\
&= \{(\partial_{\boldsymbol{F}_{\boldsymbol{\kappa}}} \psi_{\boldsymbol{\kappa}(b)}) \boldsymbol{F}_{\boldsymbol{\kappa}}^{\mathrm{T}} + (\partial_{\nabla^{\boldsymbol{\kappa}} \boldsymbol{F}_{\boldsymbol{\kappa}}} \psi_{\boldsymbol{\kappa}(b)})(\nabla^{\boldsymbol{\kappa}} \boldsymbol{F}_{\boldsymbol{\kappa}})^{\mathrm{T}}\} \cdot \boldsymbol{\Omega}\,.
\end{aligned}
\tag{20}
$$

Since $\boldsymbol{\Omega}$ is arbitrary, this implies the restriction

$$
(\partial_{\boldsymbol{F}_{\boldsymbol{\kappa}}} \psi_{\boldsymbol{\kappa}(b)}) \boldsymbol{F}_{\boldsymbol{\kappa}}^{\mathrm{T}} + (\partial_{\nabla^{\boldsymbol{\kappa}} \boldsymbol{F}_{\boldsymbol{\kappa}}} \psi_{\boldsymbol{\kappa}(b)})(\nabla^{\boldsymbol{\kappa}} \boldsymbol{F}_{\boldsymbol{\kappa}})^{\mathrm{T}} \quad \text{symmetric} \tag{21}
$$

on the derivative of $\psi_{\boldsymbol{\kappa}(b)}$ with respect to its first two arguments. This represents a direct generalization to gradient continua of the classic result (*e.g.*, Noll, 1955; Truesdell and Noll, 1992, §84) for simple materials that material frame-indifference requires the Cauchy stress, or equivalently the Kirchhoff stress to be symmetric in the hyperelastic context. Indeed, if we neglect the gradient dependence in (21), it reduces to the Kirchhoff stress $(\partial_{\boldsymbol{F}_{\boldsymbol{\kappa}}} \psi_{\boldsymbol{\kappa}(b)}) \boldsymbol{F}_{\boldsymbol{\kappa}}^{\mathrm{T}}$, at any material point b and with respect to any first-order local configuration $\nabla\boldsymbol{\kappa}(b)$. This is perhaps the most well-known example of the fact that material frame-indifference, implicating spatial isotropy, provides restrictions both on the form of constitutive relations and their derivatives. As shown by the current results (18), (19) and (21), this is true for inelastic gradient continua as well.

4 Material isomorphism

In the context of simple materials, the elastoplastic multiplicative decomposition of $\boldsymbol{F}$ has long been recognized as being perhaps the most prominant example of the modeling of $\boldsymbol{F}_{\mathrm{M}} \equiv \boldsymbol{F}_{\mathrm{P}}$ as a so-called (elastic) material isomorphism or time-dependent change of local reference placement (*e.g.*, Bertram, 1998; Svendsen, 2001; Wang and Bloom, 1974). In the current context, this represents a first-order material isomorphism. As it turns out, there is a generalization of this to the current case of second-order inelastic or inelastic gradient materials in terms of $\mathcal{F}_{\mathrm{M}}$ as based on the jet product (6). Indeed, by direct analogy, $\mathcal{F}_{\mathrm{M}}(t, b)$ represents such an isomorphism or change of local placement for b at any time $t \in I$ when there exists a reduced form $\psi_{\mathrm{i}\,b}$ of ψ_b such that

$$
\psi_b(\mathcal{F}, \mathcal{F}_{\mathrm{M}}) = \psi_{\mathcal{P}_{\boldsymbol{\kappa}}(b)}(\mathcal{F}_{\boldsymbol{\kappa}}, \mathcal{F}_{\mathrm{M}\boldsymbol{\kappa}}) = \det(\boldsymbol{F}_{\mathrm{M}\boldsymbol{\kappa}})\, \psi_{\mathrm{i}\,\mathcal{P}_{\boldsymbol{\kappa}}(b)}(\mathcal{F}_{\mathrm{E}\boldsymbol{\kappa}})\,, \tag{22}
$$

i.e.,

$$
\psi_{\boldsymbol{\kappa}(b)}(\boldsymbol{F}_{\boldsymbol{\kappa}}, \nabla^{\boldsymbol{\kappa}} \boldsymbol{F}_{\boldsymbol{\kappa}}, \boldsymbol{F}_{\mathrm{M}\boldsymbol{\kappa}}, \nabla^{\boldsymbol{\kappa}} \boldsymbol{F}_{\mathrm{M}\boldsymbol{\kappa}}) = \det(\boldsymbol{F}_{\mathrm{M}\boldsymbol{\kappa}})\, \psi_{\mathrm{i}\,\boldsymbol{\kappa}(b)}(\boldsymbol{F}_{\mathrm{E}\boldsymbol{\kappa}}, \nabla^{\mathrm{i}} \boldsymbol{F}_{\mathrm{E}\boldsymbol{\kappa}})\,, \tag{23}
$$

holds with respect to some $\mathcal{P}_{\boldsymbol{\kappa}}(b)$. Here,

$$
\begin{aligned}
\mathcal{F}_{\mathrm{E}\boldsymbol{\kappa}} &:= \mathcal{F}_{\boldsymbol{\kappa}} * \mathcal{F}_{\mathrm{M}\boldsymbol{\kappa}}^{-1} \\
&= \{\boldsymbol{F}_{\boldsymbol{\kappa}}\boldsymbol{F}_{\mathrm{M}\boldsymbol{\kappa}}^{-1}, \nabla^{\boldsymbol{\kappa}}\boldsymbol{F}_{\boldsymbol{\kappa}}[\boldsymbol{F}_{\mathrm{M}\boldsymbol{\kappa}}^{-1}, \boldsymbol{F}_{\mathrm{M}\boldsymbol{\kappa}}^{-1}] - \boldsymbol{F}_{\boldsymbol{\kappa}}\boldsymbol{F}_{\mathrm{M}\boldsymbol{\kappa}}^{-1}\nabla^{\boldsymbol{\kappa}}\boldsymbol{F}_{\mathrm{M}\boldsymbol{\kappa}}[\boldsymbol{F}_{\mathrm{M}\boldsymbol{\kappa}}^{-1}, \boldsymbol{F}_{\mathrm{M}\boldsymbol{\kappa}}^{-1}]\} \\
&= \{\boldsymbol{F}_{\mathrm{E}\boldsymbol{\kappa}}, \nabla^{\mathrm{i}}\boldsymbol{F}_{\mathrm{E}\boldsymbol{\kappa}}\}\ ,
\end{aligned} \tag{24}
$$

with

$$
\begin{aligned}
\boldsymbol{F}_{\mathrm{E}\boldsymbol{\kappa}} &:= \boldsymbol{F}_{\boldsymbol{\kappa}}\boldsymbol{F}_{\mathrm{M}\boldsymbol{\kappa}}^{-1}\ , \\
\nabla^{\mathrm{i}}\boldsymbol{F}_{\mathrm{E}\boldsymbol{\kappa}} &:= (\nabla^{\boldsymbol{\kappa}}\boldsymbol{F}_{\mathrm{E}\boldsymbol{\kappa}})\boldsymbol{F}_{\mathrm{M}\boldsymbol{\kappa}}^{-1}\ ,
\end{aligned} \tag{25}
$$

represents the second-order elastic local deformation, formally analogous to, and containing, its first order counterpart $\boldsymbol{F}_{\mathrm{E}\boldsymbol{\kappa}}$. Since

$$
\begin{aligned}
\mathcal{F}_{\mathrm{E}\boldsymbol{\kappa}} &= \mathcal{F}_{\boldsymbol{\kappa}} * \mathcal{F}_{\mathrm{M}\boldsymbol{\kappa}}^{-1} \\
&= \mathcal{F}_{\boldsymbol{\gamma}} * \mathcal{H}_{\boldsymbol{\gamma\kappa}} * \mathcal{H}_{\boldsymbol{\gamma\kappa}}^{-1} * \mathcal{F}_{\mathrm{M}\boldsymbol{\gamma}}^{-1} \\
&= \mathcal{F}_{\boldsymbol{\gamma}} * \mathcal{F}_{\mathrm{M}\boldsymbol{\gamma}}^{-1} \\
&= \mathcal{F}_{\mathrm{E}\boldsymbol{\gamma}}
\end{aligned}
$$

holds via (6) and (13), note that $\mathcal{F}_{\mathrm{E}\boldsymbol{\kappa}}$ is in fact independent of the choice of local placement. In this case, we have

$$
\det(\boldsymbol{F}_{\mathrm{M}\boldsymbol{\kappa}})\,\psi_{\mathrm{i}\,\mathcal{P}_{\boldsymbol{\kappa}}(b)}(\mathcal{F}_{\mathrm{E}\boldsymbol{\kappa}}) = \det(\nabla^{\boldsymbol{\kappa}}\boldsymbol{\gamma}(b))\ \det(\boldsymbol{F}_{\mathrm{M}\boldsymbol{\gamma}})\,\psi_{\mathrm{i}\,\mathcal{P}_{\boldsymbol{\gamma}}(b)}(\mathcal{F}_{\mathrm{E}\boldsymbol{\gamma}}) = \det(\boldsymbol{F}_{\mathrm{M}\boldsymbol{\kappa}})\,\psi_{\mathrm{i}\,\mathcal{P}_{\boldsymbol{\gamma}}(b)}(\mathcal{F}_{\mathrm{E}\boldsymbol{\kappa}})
$$

from (15) and the fact that $\boldsymbol{F}_{\mathrm{M}\boldsymbol{\kappa}}(t,b) = \boldsymbol{F}_{\mathrm{M}\boldsymbol{\gamma}}(t,b)\,\nabla^{\boldsymbol{\kappa}}\boldsymbol{\gamma}(b)$. As such,

$$
\psi_{\mathrm{i}\,\mathcal{P}_{\boldsymbol{\kappa}}(b)} = \psi_{\mathrm{i}\,\mathcal{P}_{\boldsymbol{\gamma}}(b)}
$$

follows. In other words, the form of the reduced free energy density $\psi_{\mathrm{i}\,\mathcal{P}_{\boldsymbol{\kappa}}(b)}$ is independent of the choice of local placement $\mathcal{P}_{\boldsymbol{\kappa}}(b)$.

Assume further that (second-order local) intermediate configuration is stress-free with respect to some $\mathcal{P}_{\boldsymbol{\kappa}}(b)$, *i.e.*,

$$
\psi_{\mathrm{i}\,\mathcal{P}_{\boldsymbol{\kappa}}(b)}(\mathcal{F}_{\mathrm{E}\boldsymbol{\kappa}} = \mathcal{I}) = \psi_{\mathrm{i}\,\boldsymbol{\kappa}(b)}(\boldsymbol{F}_{\mathrm{E}\boldsymbol{\kappa}} = \boldsymbol{I}, \nabla^{\mathrm{i}}\boldsymbol{F}_{\mathrm{E}\boldsymbol{\kappa}} = \boldsymbol{0}) = 0\ . \tag{26}
$$

In this case, the modeling of $\boldsymbol{F}_{\mathrm{M}}$ as a second-order material isomorphism or second-order change of local placement induces the generalization

$$
\mathcal{F} = \mathcal{F}_{\mathrm{E}} * \mathcal{F}_{\mathrm{M}} \tag{27}
$$

of the well-known elastoplastic multiplicative decomposition of the deformation gradient (*e.g.*, Lee, 1969) to the case of gradient continua. In particular, this takes the form

$$
\begin{aligned}
\boldsymbol{F}_{\boldsymbol{\kappa}} &= \boldsymbol{F}_{\mathrm{E}\boldsymbol{\kappa}}\boldsymbol{F}_{\mathrm{M}\boldsymbol{\kappa}} \\
\nabla^{\boldsymbol{\kappa}}\boldsymbol{F}_{\boldsymbol{\kappa}} &= \nabla^{\mathrm{i}}\boldsymbol{F}_{\mathrm{E}\boldsymbol{\kappa}}[\boldsymbol{F}_{\mathrm{M}\boldsymbol{\kappa}}, \boldsymbol{F}_{\mathrm{M}\boldsymbol{\kappa}}] + \boldsymbol{F}_{\mathrm{E}\boldsymbol{\kappa}}\,\nabla^{\boldsymbol{\kappa}}\boldsymbol{F}_{\mathrm{M}\boldsymbol{\kappa}}\ ,
\end{aligned} \tag{28}
$$

with respect to any local placement $\mathcal{P}_{\boldsymbol{\kappa}}(b)$ via (6). The latter relation can be rewritten in the form

$$\nabla^{\mathrm{i}}\boldsymbol{F}_{\mathrm{E}\boldsymbol{\kappa}} = \nabla^{\boldsymbol{\kappa}}\boldsymbol{F}_{\boldsymbol{\kappa}}[\boldsymbol{F}_{\mathrm{M}\boldsymbol{\kappa}}^{-1}, \boldsymbol{F}_{\mathrm{M}\boldsymbol{\kappa}}^{-1}] - \boldsymbol{F}_{\mathrm{E}\boldsymbol{\kappa}}\,\nabla^{\boldsymbol{\kappa}}\boldsymbol{F}_{\mathrm{M}\boldsymbol{\kappa}}[\boldsymbol{F}_{\mathrm{M}\boldsymbol{\kappa}}^{-1}, \boldsymbol{F}_{\mathrm{M}\boldsymbol{\kappa}}^{-1}] \tag{29}$$

for $\nabla^{\mathrm{i}}\boldsymbol{F}_{\mathrm{E}\boldsymbol{\kappa}}$ (see (24)). To examine this result more closely, it is useful to look at its symmetric and skew-symmetric parts, *i.e.*,

$$\begin{array}{rcl} \mathrm{sym}(\nabla^{\mathrm{i}}\boldsymbol{F}_{\mathrm{E}\boldsymbol{\kappa}}) & = & \mathrm{sym}\{\nabla^{\boldsymbol{\kappa}}\boldsymbol{F}_{\boldsymbol{\kappa}}[\boldsymbol{F}_{\mathrm{M}\boldsymbol{\kappa}}^{-1}, \boldsymbol{F}_{\mathrm{M}\boldsymbol{\kappa}}^{-1}]\} - \boldsymbol{F}_{\mathrm{E}\boldsymbol{\kappa}}\,\mathrm{sym}\{\nabla^{\boldsymbol{\kappa}}\boldsymbol{F}_{\mathrm{M}\boldsymbol{\kappa}}[\boldsymbol{F}_{\mathrm{M}\boldsymbol{\kappa}}^{-1}, \boldsymbol{F}_{\mathrm{M}\boldsymbol{\kappa}}^{-1}]\}\,, \\ \mathrm{skw}(\nabla^{\mathrm{i}}\boldsymbol{F}_{\mathrm{E}\boldsymbol{\kappa}}) & = & -\boldsymbol{F}_{\mathrm{E}\boldsymbol{\kappa}}\,\mathrm{skw}\{\nabla^{\boldsymbol{\kappa}}\boldsymbol{F}_{\mathrm{M}\boldsymbol{\kappa}}[\boldsymbol{F}_{\mathrm{M}\boldsymbol{\kappa}}^{-1}, \boldsymbol{F}_{\mathrm{M}\boldsymbol{\kappa}}^{-1}]\}\,. \end{array} \tag{30}$$

The second of these follows from the fact that $\mathrm{skw}(\nabla^{\boldsymbol{\kappa}}\boldsymbol{F}_{\boldsymbol{\kappa}})$, or $\mathrm{skw}\{\nabla^{\boldsymbol{\kappa}}\boldsymbol{F}_{\boldsymbol{\kappa}}[\boldsymbol{F}_{\mathrm{M}\boldsymbol{\kappa}}^{-1}, \boldsymbol{F}_{\mathrm{M}\boldsymbol{\kappa}}^{-1}]\}$, vanishes identically. Note that the axial form

$$\boldsymbol{G}_{\mathrm{r}\boldsymbol{\kappa}} := \mathrm{curl}^{\boldsymbol{\kappa}}\boldsymbol{F}_{\mathrm{M}\boldsymbol{\kappa}} = \mathrm{axs}(\nabla^{\boldsymbol{\kappa}}\boldsymbol{F}_{\mathrm{M}\boldsymbol{\kappa}}) = \mathrm{axi}(\mathrm{skw}(\nabla^{\boldsymbol{\kappa}}\boldsymbol{F}_{\mathrm{M}\boldsymbol{\kappa}})) \tag{31}$$

of $\mathrm{skw}(\nabla^{\boldsymbol{\kappa}}\boldsymbol{F}_{\mathrm{M}\boldsymbol{\kappa}})$ represents the referential dislocation tensor, and

$$\begin{array}{rcl} \boldsymbol{G}_{\mathrm{i}\boldsymbol{\kappa}} & := & \mathrm{axs}\{\nabla^{\boldsymbol{\kappa}}\boldsymbol{F}_{\mathrm{M}\boldsymbol{\kappa}}[\boldsymbol{F}_{\mathrm{M}\boldsymbol{\kappa}}^{-1}, \boldsymbol{F}_{\mathrm{M}\boldsymbol{\kappa}}^{-1}]\} \\ & = & \det(\boldsymbol{F}_{\mathrm{M}\boldsymbol{\kappa}})^{-1}\,(\mathrm{curl}^{\boldsymbol{\kappa}}\boldsymbol{F}_{\mathrm{M}\boldsymbol{\kappa}})\boldsymbol{F}_{\mathrm{M}\boldsymbol{\kappa}}^{\mathrm{T}} \\ & = & \boldsymbol{G}_{\mathrm{r}\boldsymbol{\kappa}}\,\mathrm{cof}(\boldsymbol{F}_{\mathrm{M}\boldsymbol{\kappa}}^{-1}) \end{array} \tag{32}$$

represents the intermediate dislocation tensor (Bilby *et al.*, 1955; Cermelli and Gurtin, 2001; Kröner, 1960; Levkovitch and Svendsen, 2006; Nye, 1953). As shown by $(30)_2$, this tensor is also determined by $\boldsymbol{F}_{\mathrm{E}\boldsymbol{\kappa}}^{-1}\,\mathrm{skw}(\nabla^{\mathrm{i}}\boldsymbol{F}_{\mathrm{E}\boldsymbol{\kappa}})$. As such, a dependence of the free energy density on $\boldsymbol{G}_{\mathrm{i}\boldsymbol{\kappa}}$ represents a special case of the material isomorphic form (22)-(23) of the free energy density.

At this point, it is interesting to compare the current formulation for gradient materials with microstructure with those (*e.g.*, Cermelli and Gurtin, 2001; Gurtin, 2002; Levkovitch and Svendsen, 2006; Menzel and Steinmann, 2000; Neff, 2008; Svendsen, 2002) in which the assumed free energy density is consistent with the (formal) special case

$$\psi_b = \psi_{\boldsymbol{\kappa}(b)}(\boldsymbol{F}_{\boldsymbol{\kappa}}, \boldsymbol{F}_{\mathrm{P}\boldsymbol{\kappa}}, \nabla^{\boldsymbol{\kappa}}\boldsymbol{F}_{\mathrm{P}\boldsymbol{\kappa}}) \tag{33}$$

of (10) in the current notation, *i.e.*, neglecting the dependence on $\nabla^{\boldsymbol{\kappa}}\boldsymbol{F}_{\boldsymbol{\kappa}}$. These have been considered, *e.g.*, for non-local extension of crystal plasticity. As discussed by Cermelli and Gurtin (2001) or Levkovitch and Svendsen (2006), for this class of materials, the non-tensorial nature of the transformation of $\nabla^{\boldsymbol{\kappa}}\boldsymbol{F}_{\mathrm{P}\boldsymbol{\kappa}}$ upon change of (global) reference placement leads to a dependence of this form of the free energy density on compatible (*i.e.*, curl-less) such changes interpreted as deformations. Such compatible deformations have been shown (*e.g.*, Davini, 1986; Davini and Parry, 1989) to leave crystallographic dislocation measures unchanged, representing as such "elastic" changes of local reference placement. The idea here is that the form of the free energy and other consitutive relations depending on such measures should then be invariant with respect to such changes of global reference placement, or alternatively, with respect to compatible deformations. This has lead many workers to work with the restriction

$$\psi_{\boldsymbol{\kappa}(b)}(\boldsymbol{F}_{\boldsymbol{\kappa}}, \boldsymbol{F}_{\mathrm{P}\boldsymbol{\kappa}}, \nabla^{\boldsymbol{\kappa}}\boldsymbol{F}_{\mathrm{P}\boldsymbol{\kappa}}) = \psi_{\mathrm{r}\boldsymbol{\kappa}(b)}(\boldsymbol{F}_{\boldsymbol{\kappa}}, \boldsymbol{F}_{\mathrm{P}\boldsymbol{\kappa}}, \boldsymbol{G}_{\mathrm{r}\boldsymbol{\kappa}}) \tag{34}$$

of the form (33) to one depending only on the skew-symmetric part of $\mathrm{skw}(\nabla^{\boldsymbol{\kappa}}\boldsymbol{F}_{\mathrm{M}\boldsymbol{\kappa}})$ which transforms tensorially. As shown by the current results, this is not the case for the current class of gradient materials as based on (10). Indeed, the transformation of $\mathcal{F}_{\mathrm{P}\boldsymbol{\kappa}}$ based on the second-order jet product is tensorial, facilitating a corresponding transformation (15) of the free energy density.

5 Material symmetry & isotropy

Consider next the consequences of material symmetry for the material isomorphic form (22) of (10). In the current context, then, material symmetry is formulated with respect to the intermediate local configuration. More generally, this can be formulated with respect to both the intermediate and reference configurations, as done by Neff (2008). To this end, we treat $\mathcal{F}_{\mathrm{E}} = \{\boldsymbol{F}_{\mathrm{E}}, \nabla^{\mathrm{i}}\boldsymbol{F}_{\mathrm{E}}\}$ formally as a (time-dependent) structure tensor (field). Then the free energy density, *e.g.*, in the form (23), is an isotropic function of its arguments with respect to the intermediate local configuration as induced by $\mathcal{F}_{\mathrm{M}}(t, b)$ (configuration) at any time $t \in I$.

As usual, the material symmetry of constitutive relations like (10) for the case of solid behavior is characterized by the action of $\mathrm{Orth}(V^3, V^3)$ on such relations. In particular, this action takes the form

$$\begin{aligned} i_{\boldsymbol{Q}}\psi_{\mathcal{P}_{\boldsymbol{\kappa}}(b)}(\mathcal{F}_{\boldsymbol{\kappa}}, \mathcal{F}_{\mathrm{M}\boldsymbol{\kappa}}) &= \psi_{\mathcal{P}_{\boldsymbol{\kappa}}(b)}(i_{\boldsymbol{Q}}\mathcal{F}_{\boldsymbol{\kappa}}, i_{\boldsymbol{Q}}\mathcal{F}_{\mathrm{M}\boldsymbol{\kappa}}) \\ &= \psi_{\boldsymbol{\kappa}(b)}(\boldsymbol{F}_{\boldsymbol{\kappa}}, \nabla^{\boldsymbol{\kappa}}\boldsymbol{F}_{\boldsymbol{\kappa}}, \boldsymbol{Q}\boldsymbol{F}_{\mathrm{M}\boldsymbol{\kappa}}, \boldsymbol{Q}\nabla^{\boldsymbol{\kappa}}\boldsymbol{F}_{\mathrm{M}\boldsymbol{\kappa}}) \end{aligned} \tag{35}$$

in the intermediate case. If $\mathcal{F}_{\mathrm{M}}$ is modeled as a material isomorphism, this can also be expressed in the form

$$\begin{aligned} i_{\boldsymbol{Q}}\psi_{\mathcal{P}_{\boldsymbol{\kappa}}(b)}(\mathcal{F}_{\boldsymbol{\kappa}}, \mathcal{F}_{\mathrm{M}\boldsymbol{\kappa}}) &= \det(i_{\boldsymbol{Q}}\boldsymbol{F}_{\mathrm{M}\boldsymbol{\kappa}})\, \psi_{\mathrm{i}\,\mathcal{P}_{\boldsymbol{\kappa}}(b)}(i_{\boldsymbol{Q}}\mathcal{F}_{\mathrm{E}\boldsymbol{\kappa}}) \\ &= \det(\boldsymbol{Q}\boldsymbol{F}_{\mathrm{M}\boldsymbol{\kappa}})\, \psi_{\mathrm{i}\,\boldsymbol{\kappa}(b)}(\boldsymbol{F}_{\mathrm{E}\boldsymbol{\kappa}}\boldsymbol{Q}^{\mathrm{T}}, \nabla^{\mathrm{i}}\boldsymbol{F}_{\mathrm{E}\boldsymbol{\kappa}}[\boldsymbol{Q}^{\mathrm{T}}, \boldsymbol{Q}^{\mathrm{T}}]) \end{aligned} \tag{36}$$

from (22) and (23). Assume next that $\psi_{\mathcal{P}_{\boldsymbol{\kappa}}(b)}$ is an isotropic function of its arguments with respect to the intermediate local configuration. Then

$$i_{\boldsymbol{Q}}\psi_{\mathcal{P}_{\boldsymbol{\kappa}}(b)} = \psi_{\mathcal{P}_{\boldsymbol{\kappa}}(b)} \tag{37}$$

holds. This implies

$$\psi_{\boldsymbol{\kappa}(b)}(\boldsymbol{F}_{\boldsymbol{\kappa}}, \nabla^{\boldsymbol{\kappa}}\boldsymbol{F}_{\boldsymbol{\kappa}}, \boldsymbol{F}_{\mathrm{M}\boldsymbol{\kappa}}, \nabla^{\boldsymbol{\kappa}}\boldsymbol{F}_{\mathrm{M}\boldsymbol{\kappa}}) = \psi_{\boldsymbol{\kappa}(b)}(\boldsymbol{F}_{\boldsymbol{\kappa}}, \nabla^{\boldsymbol{\kappa}}\boldsymbol{F}_{\boldsymbol{\kappa}}, \boldsymbol{Q}\boldsymbol{F}_{\mathrm{M}\boldsymbol{\kappa}}, \boldsymbol{Q}\nabla^{\boldsymbol{\kappa}}\boldsymbol{F}_{\mathrm{M}\boldsymbol{\kappa}}) \tag{38}$$

for all $\boldsymbol{Q} \in \mathrm{Orth}(V^3, V^3)$ in general, or alternatively

$$\psi_{\boldsymbol{\kappa}(b)}(\boldsymbol{F}_{\boldsymbol{\kappa}}, \nabla^{\boldsymbol{\kappa}}\boldsymbol{F}_{\boldsymbol{\kappa}}, \boldsymbol{F}_{\mathrm{M}\boldsymbol{\kappa}}, \nabla^{\boldsymbol{\kappa}}\boldsymbol{F}_{\mathrm{M}\boldsymbol{\kappa}}) = \det(\boldsymbol{Q}\boldsymbol{F}_{\mathrm{M}\boldsymbol{\kappa}})\, \psi_{\mathrm{i}\,\boldsymbol{\kappa}(b)}(\boldsymbol{F}_{\mathrm{E}\boldsymbol{\kappa}}\boldsymbol{Q}^{\mathrm{T}}, \nabla^{\mathrm{i}}\boldsymbol{F}_{\mathrm{E}\boldsymbol{\kappa}}[\boldsymbol{Q}^{\mathrm{T}}, \boldsymbol{Q}^{\mathrm{T}}]) \tag{39}$$

for all $\boldsymbol{Q} \in \mathrm{Orth}(V^3, V^3)$ in the case that $\mathcal{F}_{\mathrm{M}}$ is modeled as a material isomorphism. Proceeding now by formal analogy with the case of material frame-indifference, the fact that these relations holds for all orthogonal transformations implies that they do so in particular with respect to any curve $\boldsymbol{Q}(s) = \exp(\boldsymbol{\Omega}\, s)$ in $\mathrm{Orth}(V^3, V^3)$ generated by the skew-symmetric tensor $\boldsymbol{\Omega} \in \mathrm{Skw}(V^3, V^3)$. Substituting this form for $\boldsymbol{Q}$ into this last result, taking the derivative of the result with respect to s, and setting $s = 0$, one obtains

$$\begin{aligned} 0 &= \partial_{\boldsymbol{Q}(0)} \psi_{\mathcal{P}_{\boldsymbol{\kappa}}(b)} \cdot \boldsymbol{Q}'(0) \\ &= \partial_{\mathcal{F}_{\mathrm{M}\boldsymbol{\kappa}}} \psi_{\mathcal{P}_{\boldsymbol{\kappa}}(b)} \cdot i_{\boldsymbol{\Omega}} \mathcal{F}_{\mathrm{M}\boldsymbol{\kappa}} \\ &= \{(\partial_{\boldsymbol{F}_{\mathrm{M}\boldsymbol{\kappa}}} \psi_{\boldsymbol{\kappa}(b)}) \boldsymbol{F}_{\mathrm{M}\boldsymbol{\kappa}}^{\mathrm{T}} + (\partial_{\nabla^{\boldsymbol{\kappa}} \boldsymbol{F}_{\mathrm{M}\boldsymbol{\kappa}}} \psi_{\boldsymbol{\kappa}(b)})(\nabla^{\boldsymbol{\kappa}} \boldsymbol{F}_{\mathrm{M}\boldsymbol{\kappa}})^{\mathrm{T}}\} \cdot \boldsymbol{\Omega} \,. \end{aligned} \tag{40}$$

Since $\boldsymbol{\Omega}$ is arbitrary, this implies the differential restriction

$$(\partial_{\boldsymbol{F}_{\mathrm{M}\boldsymbol{\kappa}}} \psi_{\boldsymbol{\kappa}(b)}) \boldsymbol{F}_{\mathrm{M}\boldsymbol{\kappa}}^{\mathrm{T}} + (\partial_{\nabla^{\boldsymbol{\kappa}} \boldsymbol{F}_{\mathrm{M}\boldsymbol{\kappa}}} \psi_{\boldsymbol{\kappa}(b)})(\nabla^{\boldsymbol{\kappa}} \boldsymbol{F}_{\mathrm{M}\boldsymbol{\kappa}})^{\mathrm{T}} \quad \text{symmetric} \tag{41}$$

on the form of $\psi_{\boldsymbol{\kappa}(b)}$. Analogously, in the case that $\mathcal{F}_{\mathrm{M}}$ is modeled as a material isomorphism, (39) implies the differential restriction

$$\boldsymbol{F}_{\mathrm{E}\boldsymbol{\kappa}}^{\mathrm{T}} (\partial_{\boldsymbol{F}_{\mathrm{E}\boldsymbol{\kappa}}} \psi_{\mathrm{i}\,\boldsymbol{\kappa}(b)}) + (\nabla^{\boldsymbol{\kappa}} \boldsymbol{F}_{\mathrm{E}\boldsymbol{\kappa}})^{\mathrm{T}} (\partial_{\nabla^{\boldsymbol{\kappa}} \boldsymbol{F}_{\mathrm{E}\boldsymbol{\kappa}}} \psi_{\mathrm{i}\,\boldsymbol{\kappa}(b)}) \quad \text{symmetric} \tag{42}$$

on the form of $\psi_{\mathrm{i}\,\boldsymbol{\kappa}(b)}$. Again, note the formal analogy here with the differential restriction (21) on the free energy density in the case of material frame-indifference. Note also that if we neglect the gradient dependence, (41) and (42) reduce to the symmetry of $-(\partial_{\boldsymbol{F}_{\mathrm{M}\boldsymbol{\kappa}}} \psi_{\boldsymbol{\kappa}(b)}) \boldsymbol{F}_{\mathrm{M}\boldsymbol{\kappa}}^{\mathrm{T}} = \boldsymbol{F}_{\mathrm{E}\boldsymbol{\kappa}}^{\mathrm{T}} (\partial_{\boldsymbol{F}_{\mathrm{E}\boldsymbol{\kappa}}} \psi_{\mathrm{i}\,\boldsymbol{\kappa}(b)})$. Consequently, this represents a direct generalization to inelastic gradient continua of the result (Svendsen, 2001) for simple inelastic materials that the stress measure[4] thermodynamically-conjugate to $\boldsymbol{L}_{\mathrm{M}} \equiv \boldsymbol{L}_{\mathrm{P}}$ is symmetric when the free energy density is an isotropic function of its arguments with respect to the intermediate local configuration.

6 Thermodynamic & configurational field relations

Up to this point, we have discussed issues pertaining to the material behavior of a single material point $b \in B$. Now the question arises as to whether or not the material points of B all represent the "same material." In other words, whether or not the behavior of each $b \in B$ is described by the same form of ψ_b. If this is not the case, the material is heterogeneous or inhomogeneous, and one speaks of material inhomogeneity (*e.g.*, Epstein and Elźanowski, 2007; Noll, 1967; Šilhavý, 1997; Truesdell and Noll, 1992). An abstract means of characterizing whether or not two material points represent the same material is that of a material uniformity (Epstein and Elźanowski, 2007; Noll, 1967). This has been shown to be related to the formulation of the Eshelby stress in the elastic (*e.g.*, Maugin, 1993) and inelastic (*e.g.*, Svendsen, 2001) context.

More recently, the focus has shifted away from the abstraction of material inhomogeneity or uniformity and onto Eshelby or configurational mechanics (*e.g.*, Gurtin, 2000; Maugin, 1993). As in the classical special case of the J-integral, the formulation of the Eshelby stress and configurational force balance are, strictly-speaking, restricted to models admitting (stress) potentials. As such, the incremental variational approach of (*e.g.*, Carstensen et al., 2003; Miehe, 2002; Ortiz and Repetto, 1999) and corresponding incremental stress potential provides a means to generalize the formulation of configuration fields and balance relations to the case of inelastic, history-dependent material

[4]Sometimes referred to as the Mandel stress (Mandel, 1971), but this is a matter of convention.

models (Svendsen, 2005). The physical basis of this approach is the continuum thermodynamic field formulation of such models as based on a rate potential (*e.g.*, Svendsen, 2004), representing the sum of the energy storage rate and dissipation potential. The purpose of this last section is to apply this approach to the current formulation of gradient materials with microstructure.

As stated above, the coupled-field problem here involves the deformation $\boldsymbol{\chi}$ and inelastic local deformation $\boldsymbol{F}_{\rm M}$ fields as basic unknowns. Restricting attention for simplicity to isothermal and quasi-static conditions, as well as smooth fields, the entropy balance for such a material takes the form[5]

$$\int_{\boldsymbol{\kappa}} \dot{\psi}_{\boldsymbol{\kappa}} + \delta_{\boldsymbol{\kappa}} = \int_{\partial\boldsymbol{\kappa}} \boldsymbol{t}_{\boldsymbol{\kappa}} \cdot \dot{\boldsymbol{\chi}}_{\boldsymbol{\kappa}} + \boldsymbol{M}_{\boldsymbol{\kappa}} \cdot \nabla^{\boldsymbol{\kappa}} \dot{\boldsymbol{\chi}}_{\boldsymbol{\kappa}} + \boldsymbol{\Phi}_{{\rm M}\boldsymbol{\kappa}} \cdot \dot{\boldsymbol{F}}_{{\rm M}\boldsymbol{\kappa}} \tag{43}$$

integrated over the reference configuration $B_{\boldsymbol{\kappa}}$ in terms of the dissipation-rate density $\delta_{\boldsymbol{\kappa}}$, boundary traction $\boldsymbol{t}_{\boldsymbol{\kappa}}$, boundary traction moment $\boldsymbol{M}_{\boldsymbol{\kappa}}$, and boundary flux $\boldsymbol{\Phi}_{{\rm M}\boldsymbol{\kappa}}$ associated with $\dot{\boldsymbol{F}}_{{\rm M}\boldsymbol{\kappa}}$. As shown in Svendsen (2004, 2005), the variational formulation of balance and consitutive relations emanating as restrictions from the dissipation principle as based on (43) can be formulated variationally as a minimization problem in terms of a dissipation potential $d_{\mathcal{P}_{\boldsymbol{\kappa}}}$ and corresponding rate potential

$$r_{\mathcal{P}_{\boldsymbol{\kappa}}}(\mathcal{F}_{\boldsymbol{\kappa}}, \mathcal{F}_{{\rm M}\boldsymbol{\kappa}}, \dot{\mathcal{F}}_{\boldsymbol{\kappa}}, \dot{\mathcal{F}}_{{\rm M}\boldsymbol{\kappa}}, b) := \dot{\psi}_{\mathcal{P}_{\boldsymbol{\kappa}}}(\mathcal{F}_{\boldsymbol{\kappa}}, \mathcal{F}_{{\rm M}\boldsymbol{\kappa}}, \dot{\mathcal{F}}_{\boldsymbol{\kappa}}, \dot{\mathcal{F}}_{{\rm M}\boldsymbol{\kappa}}, b) + d_{\mathcal{P}_{\boldsymbol{\kappa}}}(\mathcal{F}_{\boldsymbol{\kappa}}, \mathcal{F}_{{\rm M}\boldsymbol{\kappa}}, \dot{\mathcal{F}}_{\boldsymbol{\kappa}}, \dot{\mathcal{F}}_{{\rm M}\boldsymbol{\kappa}}, b)\ . \tag{44}$$

Integrating this over the reference configuration and taking its first variation, we obtain

$$\begin{aligned}
\delta \int_{\boldsymbol{\kappa}} r_{\boldsymbol{\kappa}} &= \int_{\boldsymbol{\kappa}} \partial_{\nabla^{\kappa}\dot{\boldsymbol{\chi}}} r_{\boldsymbol{\kappa}} \cdot \nabla^{\boldsymbol{\kappa}} \delta\dot{\boldsymbol{\chi}} + \partial_{\nabla^{\kappa}\nabla^{\kappa}\dot{\boldsymbol{\chi}}} r_{\boldsymbol{\kappa}} \cdot \nabla^{\boldsymbol{\kappa}}\nabla^{\boldsymbol{\kappa}} \delta\dot{\boldsymbol{\chi}} + \partial_{\dot{\boldsymbol{F}}_{{\rm M}\boldsymbol{\kappa}}} r_{\boldsymbol{\kappa}} \cdot \delta\dot{\boldsymbol{F}}_{{\rm M}\boldsymbol{\kappa}} + \partial_{\nabla^{\kappa}\dot{\boldsymbol{F}}_{{\rm M}\boldsymbol{\kappa}}} r_{\boldsymbol{\kappa}} \cdot \delta\, \nabla^{\boldsymbol{\kappa}} \dot{\boldsymbol{F}}_{{\rm M}\boldsymbol{\kappa}} \\
&= \int_{\partial\boldsymbol{\kappa}} \boldsymbol{t}_{\boldsymbol{\kappa}} \cdot \delta\dot{\boldsymbol{\chi}}_{\boldsymbol{\kappa}} + \boldsymbol{M}_{\boldsymbol{\kappa}} \cdot \delta\nabla^{\boldsymbol{\kappa}}\dot{\boldsymbol{\chi}}_{\boldsymbol{\kappa}} + \boldsymbol{\Phi}_{{\rm M}\boldsymbol{\kappa}} \cdot \delta\dot{\boldsymbol{F}}_{{\rm M}\boldsymbol{\kappa}}\ .
\end{aligned} \tag{45}$$

Integration by parts und application of the divergence theorem then yield

$$\begin{aligned}
0 &= \int_{\partial\boldsymbol{\kappa}} \{\boldsymbol{t}_{\boldsymbol{\kappa}} - (\delta_{\nabla^{\kappa}\dot{\boldsymbol{\chi}}} r_{\boldsymbol{\kappa}})\boldsymbol{n}_{\boldsymbol{\kappa}}\} \cdot \delta\dot{\boldsymbol{\chi}} + \{\boldsymbol{M}_{\boldsymbol{\kappa}} - (\partial_{\nabla^{\kappa}\nabla^{\kappa}\dot{\boldsymbol{\chi}}} r_{\boldsymbol{\kappa}})\boldsymbol{n}_{\boldsymbol{\kappa}}\} \cdot \delta\nabla^{\boldsymbol{\kappa}}\dot{\boldsymbol{\chi}} \\
&+ \int_{\partial\boldsymbol{\kappa}} \{\boldsymbol{\Phi}_{{\rm M}\boldsymbol{\kappa}} - (\partial_{\nabla^{\kappa}\dot{\boldsymbol{F}}_{{\rm M}\boldsymbol{\kappa}}} r_{\boldsymbol{\kappa}})\boldsymbol{n}_{\boldsymbol{\kappa}}\} \cdot \delta\dot{\boldsymbol{F}}_{{\rm M}\boldsymbol{\kappa}} \\
&+ \int_{\boldsymbol{\kappa}} {\rm div}^{\boldsymbol{\kappa}}(\delta_{\nabla^{\kappa}\dot{\boldsymbol{\chi}}} r_{\boldsymbol{\kappa}}) \cdot \delta\dot{\boldsymbol{\chi}} - \delta_{\dot{\boldsymbol{F}}_{{\rm M}\boldsymbol{\kappa}}} r_{\boldsymbol{\kappa}} \cdot \delta\dot{\boldsymbol{F}}_{{\rm M}\boldsymbol{\kappa}}
\end{aligned} \tag{46}$$

in terms of the variational derivative

$$\delta_x f := \partial_x f - {\rm div}(\partial_{\nabla x} f)\ . \tag{47}$$

From this, we obtain the necessary field relations

$$\begin{aligned}
{\rm div}^{\boldsymbol{\kappa}}(\delta_{\nabla^{\kappa}\dot{\boldsymbol{\chi}}} r_{\boldsymbol{\kappa}}) &= \boldsymbol{0}\ , \\
\delta_{\dot{\boldsymbol{F}}_{{\rm M}\boldsymbol{\kappa}}} r_{\boldsymbol{\kappa}} &= \boldsymbol{0}\ ,
\end{aligned} \tag{48}$$

[5]We dispense with the surface da and volume dv elements in the corresponding integrals in what follows for notational simplicity.

on $B_{\boldsymbol{\kappa}}$ and boundary conditions

$$
\begin{aligned}
\boldsymbol{t}_{\boldsymbol{\kappa}} &= (\delta_{\nabla^{\boldsymbol{\kappa}}\dot{\boldsymbol{\chi}}} r_{\boldsymbol{\kappa}})\boldsymbol{n}_{\boldsymbol{\kappa}} \,, \\
\boldsymbol{M}_{\boldsymbol{\kappa}} &= (\partial_{\nabla^{\boldsymbol{\kappa}}\nabla^{\boldsymbol{\kappa}}\dot{\boldsymbol{\chi}}} r_{\boldsymbol{\kappa}})\boldsymbol{n}_{\boldsymbol{\kappa}} \,, \\
\boldsymbol{\Phi}_{\mathrm{M}\boldsymbol{\kappa}} &= (\partial_{\nabla^{\boldsymbol{\kappa}}\dot{\boldsymbol{F}}_{\mathrm{M}\boldsymbol{\kappa}}} r_{\boldsymbol{\kappa}})\boldsymbol{n}_{\boldsymbol{\kappa}} \,,
\end{aligned}
\tag{49}
$$

on the flux part of $\partial B_{\boldsymbol{\kappa}}$. In particular, $(48)_1$ represents a generalization to the current rate context of the standard extended momentum balance for a Mindlin or strain-gradient continuum (*e.g.*, Fleck and Hutchinson, 1997; Neff *et al.*, 2008). Furthermore, $(48)_2$ represents a rate-based generalization of a Cahn-Allen-type field relation for $\boldsymbol{F}_{\mathrm{M}\boldsymbol{\kappa}}$, identifying it in this context as a type of tensor-valued phase field.

With this basic continuum thermodynamic variational formulation in hand, we are now in a position to obtain its incremental variational form. This is based on the corresponding incremental form

$$
\begin{aligned}
& w_{\boldsymbol{\kappa}e,s}(\boldsymbol{F}_{\boldsymbol{\kappa}e}, \nabla^{\boldsymbol{\kappa}}\boldsymbol{F}_{\boldsymbol{\kappa}e}, \boldsymbol{F}_{\mathrm{M}\boldsymbol{\kappa}e}, \nabla^{\boldsymbol{\kappa}}\boldsymbol{F}_{\mathrm{M}\boldsymbol{\kappa}e}, \boldsymbol{\kappa}(b)) \\
&:= \int_{t_s}^{t_e} r_{\boldsymbol{\kappa}} \\
&= \psi_{\boldsymbol{\kappa}e}(\boldsymbol{F}_{\boldsymbol{\kappa}e}, \nabla^{\boldsymbol{\kappa}}\boldsymbol{F}_{\boldsymbol{\kappa}e}, \boldsymbol{F}_{\mathrm{M}\boldsymbol{\kappa}e}, \nabla^{\boldsymbol{\kappa}}\boldsymbol{F}_{\mathrm{M}\boldsymbol{\kappa}e}, \boldsymbol{\kappa}(b)) - \psi_{\boldsymbol{\kappa}s} + \int_{t_s}^{t_e} d_{\boldsymbol{\kappa}} \\
&= \psi_{\boldsymbol{\kappa}e}(\boldsymbol{F}_{\boldsymbol{\kappa}e}, \nabla^{\boldsymbol{\kappa}}\boldsymbol{F}_{\boldsymbol{\kappa}e}, \boldsymbol{F}_{\mathrm{M}\boldsymbol{\kappa}e}, \nabla^{\boldsymbol{\kappa}}\boldsymbol{F}_{\mathrm{M}\boldsymbol{\kappa}e}, \boldsymbol{\kappa}(b)) - \psi_{\boldsymbol{\kappa}s} \\
&\quad + t_{e,s}\, d_{\boldsymbol{\kappa}e,s}(\boldsymbol{F}_{\boldsymbol{\kappa}e}, \nabla^{\boldsymbol{\kappa}}\boldsymbol{F}_{\boldsymbol{\kappa}e}, \boldsymbol{F}_{\mathrm{M}\boldsymbol{\kappa}e}, \nabla^{\boldsymbol{\kappa}}\boldsymbol{F}_{\mathrm{M}\boldsymbol{\kappa}e}, \boldsymbol{\kappa}(b))
\end{aligned}
\tag{50}
$$

of $r_{\boldsymbol{\kappa}}$ obtained via time-integration over a finite time-interval $[t_s, t_e]$ of duration $t_{e,s} := t_e - t_s$, with

$$
\begin{aligned}
& d_{\boldsymbol{\kappa}e,s}(\boldsymbol{F}_{\boldsymbol{\kappa}e}, \nabla^{\boldsymbol{\kappa}}\boldsymbol{F}_{\boldsymbol{\kappa}e}, \boldsymbol{F}_{\mathrm{M}\boldsymbol{\kappa}e}, \nabla^{\boldsymbol{\kappa}}\boldsymbol{F}_{\mathrm{M}\boldsymbol{\kappa}e}, \boldsymbol{\kappa}(b)) \\
&:= d_{\boldsymbol{\kappa}}\left(\boldsymbol{F}_{\boldsymbol{\kappa}s}, \nabla^{\boldsymbol{\kappa}}\boldsymbol{F}_{\boldsymbol{\kappa}s}, \boldsymbol{F}_{\mathrm{M}\boldsymbol{\kappa}s}, \nabla^{\boldsymbol{\kappa}}\boldsymbol{F}_{\mathrm{M}\boldsymbol{\kappa}s}, \frac{\boldsymbol{F}_{\boldsymbol{\kappa}e,s}}{t_{e,s}}, \frac{\nabla^{\boldsymbol{\kappa}}\boldsymbol{F}_{\boldsymbol{\kappa}e,s}}{t_{e,s}}, \frac{\boldsymbol{F}_{\mathrm{M}\boldsymbol{\kappa}e,s}}{t_{e,s}}, \frac{\nabla^{\boldsymbol{\kappa}}\boldsymbol{F}_{\mathrm{M}\boldsymbol{\kappa}e,s}}{t_{e,s}}, \boldsymbol{\kappa}(b)\right)
\end{aligned}
\tag{51}
$$

the corresponding form of the dissipation potential. Note that we have chosen explicit or forward-Euler time-integration in the process for simplicity; implicit or backward-Euler integration is also possible (*e.g.*, Carstensen et al., 2003; Miehe, 2002). In this later case, however, one must take care to preserve the potential structure of the incremental formulation. Since the dissipation potential is necessarily convex in its rate arguments, *i.e.*, in order to satisfy the dissipation principle (*i.e.*, sufficiently), this is automatically given in the explicit approach considered here.

Given the form (51) of the incremental potential, application of the approach in Svendsen (2005) to the formulation of configurational fields and balance relations yields the result

$$
\mathbf{0} = \mathrm{div}^{\boldsymbol{\kappa}}\boldsymbol{E}_{\boldsymbol{\kappa}e,s} - \partial_{\boldsymbol{\kappa}} w_{\boldsymbol{\kappa}e,s}
\tag{52}
$$

for the (now incremental) generalized configurational force balance as based on the corresponding form

$$
\boldsymbol{E}_{\boldsymbol{\kappa}e,s} = w_{\boldsymbol{\kappa}e,s}\boldsymbol{I} - (\nabla^{\boldsymbol{\kappa}}\boldsymbol{\chi}_e)^{\mathrm{T}}(\partial_{\nabla^{\boldsymbol{\kappa}}\boldsymbol{\chi}_e} w_{\boldsymbol{\kappa}e,s}) - (\nabla^{\boldsymbol{\kappa}}\boldsymbol{F}_{\mathrm{M}\boldsymbol{\kappa}e})^{\mathrm{T}}(\partial_{\nabla^{\boldsymbol{\kappa}}\boldsymbol{F}_{\mathrm{M}\boldsymbol{\kappa}e}} w_{\boldsymbol{\kappa}e,s})
\tag{53}
$$

of the (incremental) Eshelby stress. Again, both of these represent generalizations to the case of history-dependent behavior. This fact is expressed explicitly in the form of $\boldsymbol{E}_{\boldsymbol{\kappa}e,s}$ via its dependence on the third term. Furthermore, if both the free energy and dissipation potential are objective-isotropic functions of their arguments as discussed above, it will be symmetric. As in the general case, material inhomogeneity appears in the configurational force balance (52) in the guise of the source term $\partial_{\boldsymbol{\kappa}} w_{\boldsymbol{\kappa}e,s}$ due to the assumed inhomogeneity of the material response. Material homogeneity would imply translational invariance of this response. In this latter case, $\partial_{\boldsymbol{\kappa}} w_{\boldsymbol{\kappa}e,s}$ vanishes, and the configurational force balance is equivalent to the Eshelby stress being a null Lagrangian (*e.g.*, Olver, 1986; Šilhavý, 1997).

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