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RESEARCH PAPER

Thermodynamic and rate variational formulation of models for inhomogeneous gradient materials with microstructure and application to phase field modeling

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Abstract In this work, thermodynamic models for the energetics and kinetics of inhomogeneous gradient materials with microstructure are formulated in the context of continuum thermodynamics and material theory. For simplicity, attention is restricted to isothermal conditions. The materials of interest here are characterized by (1) first- and second-order gradients of the deformation field and (2) a kinematic microstructure field and its gradient (e.g., in the sense of director, micromorphic or Cosserat microstructure). Material inhomogeneity takes the form of multiple phases and chemical constituents, modeled here with the help of corresponding phase fields. Invariance requirements together with the dissipation principle result in the reduced model field and constitutive relations. Special cases of these include the well-known Cahn–Hilliard and Ginzburg–Landau relations. In the last part of the work, initial boundary value problems for this class of materials are formulated with the help of rate variational methods.

Keywords Continuum thermodynamics · Material inhomogeneity · Conservative · Non-conservative phase fields

1 Introduction

Among the most basic assumptions of standard macroscopic phenomenological material theory are those of "simple" material behavior and homogeneity of material properties (e.g., [1–3]). As witnessed by the vast literature that has accumulated on the subject in the last decades (e.g., [4–9]), both of these assumptions are questionable for an ever increasing variety of engineering materials and systems whose material properties and behavior are strongly influenced by a material microstructure, resulting material length- and timescale dependence, and material heterogeneity. This state of affairs is certainly one reason for the concomitant development and increasingly wide-spread application of modeling methods such as statistical and homogenization methods (e.g., [6–10]), Eshelby or configurational mechanics (e.g., [9,11,12]), or phase field methods [4,13–18].

In the theoretical continuum mechanics community, generalizations of the lengthscale-less concept of simple material behavior were of interest quite early on. The simplest of these is the notion of (non-simple) elastic higher-order continua (e.g., [19–22]) in which the material behavior depends on second- and/or higher-order gradients of the continuum deformation field. The idea here is that the region of influence of neighboring material points on the behavior of a given material point increases with increasing intrinsic material heterogeneity, leading to a loss of local action [1], something which happens as the system size approaches that of the microstructure. Another class of such generalizations involves the introduction of one or more fields besides the continuum deformation field, which represent in a strongly idealized "mean-field" fashion the effect of microstructure which evolves relative to the continuum. Prominent examples include Cosserat [23] and micropolar (e.g., [24,25]) continua, general oriented continua, micromorphic continua (e.g., [26,27]), director models for anisotropic fluids and liquid crystals (e.g., [28–30]), or mod-

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els for porous materials (e.g., [31]). All of these may be categorized under the rubric of elastic continua with elastic microstructure (e.g., [32–34]). The literature on extended or generalized continua in this sense spans more than 100 years; for reviews on this work, see Ref. [1] (before 1965) or more recently [35], celebrating 100 years of Cosserat theory.

Both of these generalizations, i.e., the generalization to gradient continua, and that to continua with microstructure, are of interest in the current work as well. In particular, homogeneous second-order continua in the sense of Refs. [22,36] and homogeneous continua with (kinematic) microstructure in the sense of Refs. [32,36], are generalized here to large deformation and heterogeneous material properties. In contrast, for example, to Refs. [22,36], however, this is not done by working with variational principles and special variations from the start. Rather, in the spirit of, for example, Refs. [2,3,19,20,32,37,38], this is carried out here in the framework of continuum thermodynamics, the energy balance, the dissipation principle, and invariance arguments. In this framework, the basic physical assumption is that both higher-order "Mindlin" stresses and microstructure evolution result in an additional flux and supply of energy in the material. On this basis, evolution-field relations for the microstructure fields may be formulated with the help of (Euclidean) frame-indifference requirements, e.g., on the total rate of work [32], or more generally, on the total energy balance (e.g., [38]). Following this latter approach, reduced balance, field and constitutive relations for homogeneous gradient continua with microstructure satisfying energy balance, the dissipation principle, and indifference requirements were obtained recently by Ref. [39].

In continuum mechanics and material theory, the separate, but related issue of heterogeneous material properties is one focus of the development of Eshelby mechanics and the concept of material or configurational forces (e.g., [9,11,12]), and at a more abstract level, the concept of material uniformity [2,40]. Perhaps the most well-known example of such a uniformity in material science and mechanics is the notion of a phase field [4,13–15,17,18]. In the current work, models for the energetics and kinetics of homogeneous gradient continua with microstructure are generalized to the case that the material in question contains multiple chemical constituents and structural (solid) phases. These are modeled by corresponding phase fields, i.e., partial mass densities and structural order parameters.

As demonstrated in a number of previous works [39,41,42], given reduced balance, field and constitutive relations based on models for the free energy (energetics) and dissipation potential (kinetics), one is in a position to formulate the corresponding initial boundary value problem (IBVP) in rate variational form. As shown, for example, in Refs. [43,44], via numerical time integration, the general rate variational form of the IBVP can be recast into a numerical time incremental form. This latter form is directly applicable to the algorithmic formulation of models for generalized and inelastic continua (e.g., multifield models, phase-field models, gradient plasticity).

The current work begins (Sect. 2) with a brief summary of the basic balance and thermodynamic relations for (chemically and structurally) heterogeneous gradient continua with microstructure. In particular, these include mass balance relations for the chemical constituents, the total energy balance, and the dissipation-rate density, for the current material class. This is followed (Sect. 3) by exploitation of the Euclidean frame-indifference of the total energy balance and dissipation rate to obtained reduced frame-indifferent (coupled) balance relations for continuum and microstructure momentum. Given basic and reduced balance relations, the current treatment turns next to energetics (Sect. 4) and kinetics (Sect. 5), the latter in the context of the dissipation principle. Assuming in particular that the kinetic relations can be derived from a dissipation potential, the reduced balance and constitutive relations may be cast in rate variational form (Sect. 6). These in turn represent the basis for the rate variational formulation of the corresponding IBVP (Sect. 7). The work ends with a discussion (Sect. 8).

The current work employs the following notation. Euclidean vectors and second-order tensors, or corresponding fields, are denoted by lower-case $\boldsymbol{a}, \boldsymbol{b}, \ldots$ and upper-case $\boldsymbol{A}, \boldsymbol{B}, \ldots$ bold italic letters. In particular, $\boldsymbol{I}$ represents the second-order identity tensor. As usual, let $\boldsymbol{a}\cdot\boldsymbol{b}$ and $\boldsymbol{a}\otimes\boldsymbol{b}$ represent the scalar and tensor product, respectively, of any two vectors $\boldsymbol{a}, \boldsymbol{b}$, with $(\boldsymbol{a}\otimes\boldsymbol{b})\,\boldsymbol{c} := (\boldsymbol{b}\cdot\boldsymbol{c})\,\boldsymbol{a}$. Also, $\boldsymbol{A}^{\mathrm{T}}\boldsymbol{a}\cdot\boldsymbol{b} := \boldsymbol{a}\cdot\boldsymbol{A}\boldsymbol{b}$ defines the transpose $\boldsymbol{A}^{\mathrm{T}}$, and $\operatorname{skw}\boldsymbol{A} := \frac{1}{2}(\boldsymbol{A} - \boldsymbol{A}^{\mathrm{T}})$ the skew-symmetric part, of any $\boldsymbol{A}$. Third-order tensors and tensor fields are denoted by upper case sans-serif characters A, B, and so on. Note that the second-order gradient $\nabla\nabla\boldsymbol{v}$ of any vector field $\boldsymbol{v}$, or the gradient $\nabla\boldsymbol{T}$ of any second-order tensor field $\boldsymbol{T}$, are third-order tensor fields. The scalar product of two tensors $\mathcal{A}, \mathcal{B}$ of equal, but otherwise arbitrary order is denoted by the order-independent notation $\mathcal{A}\cdot\mathcal{B}$ in this work. Given this, the direct tensor product $\mathcal{A}\otimes\mathcal{B}$ is defined by $(\mathcal{A}\otimes\mathcal{B})\,\mathcal{C} := (\mathcal{B}\cdot\mathcal{C})\,\mathcal{A}$. Additional such concepts and definitions will be introduced as needed along the way.

2 Basic relations

For simplicity, attention is restricted in the current work to the case of isothermal elasticity; for treatment of inelastic homogeneous gradient materials with microstructure, the reader is referred to Refs. [39,42]. The model formulation to follow is for finite deformation, and all fields are referen-

tial or "Lagrangian". The class of continua with kinematic microstructure under consideration here is characterized in particular by a pair $(\boldsymbol{\chi}, \boldsymbol{\varsigma})$ of continuum fields. Here, $\boldsymbol{\chi}$ is the macroscopic (mean) deformation field, and $\boldsymbol{\varsigma}$ is a kinematic microstructural field whose evolution influences the macroscopic behavior. For example, $\boldsymbol{\varsigma}$ could represent a vector field (e.g., director field), or a tensor field (e.g., Cosserat or micropolar local rotation, micromorphic local deformation). As stated in the introduction, material inhomogeneity in the current work is due to presence of $m+1$ chemical (mass) constituents or components, and p spatially distinct (solid) phases, in the material. In the phase field approach (e.g., [4,17,45]), the latter are modeled by corresponding (non-conservative) structural order parameters $\phi_1, \dots, \phi_p$, and the former by (conservative) "partial" mass densities $\varrho_1, \dots, \varrho_{m+1}$ (i.e., constituent mass per unit reference volume). Let ϱ_a represent the "partial" mass density of constituent $a = 1, \dots, m+1$, and ϱ the referential mass density of the material as a whole (mixture). Constituent mass balance then takes the form

$$\dot{\varrho}_a + \operatorname{div} \boldsymbol{j}_a = \sigma_a \tag{1}$$

in terms of the constituent mass flux density $\boldsymbol{j}_a$ and corresponding supply rate density σ_a in the reference configuration. Since mass is additive,

$$\varrho = \sum_{a=1}^{m+1} \varrho_a \tag{2}$$

holds, and so

$$\dot{\varrho} + \operatorname{div} \sum_{a=1}^{m+1} \boldsymbol{j}_a = \sum_{a=1}^{m+1} \sigma_a . \tag{3}$$

In this work, we assume that the continuum under consideration is a closed system with respect to mass, i.e.,

$$\sum_{a=1}^{m+1} \boldsymbol{j}_a = \boldsymbol{0} , \quad \sum_{a=1}^{m+1} \sigma_a = 0 . \tag{4}$$

Then $\dot{\varrho}$ vanishes, and ϱ is constant in time. In this case,

$$\varrho_{m+1} = \varrho - \sum_{a=1}^{m} \varrho_a \tag{5}$$

is determined by ϱ and $\boldsymbol{\varrho} = (\varrho_1, \dots, \varrho_m)$, and only m of the ϱ_a are independent.

As mentioned above, for simplicity, the following treatment is restricted to isothermal processes. Also, all processes are assumed for simplicity to be continuous and continuously differentiable in space and time, which excludes, for example, singular surfaces. On this basis, the general form

$$\mathcal{E} = \overline{\int_B f}^{\cdot} + \int_B \delta - \int_B s - \int_{\partial B} \boldsymbol{f} \cdot \boldsymbol{n} = 0 \tag{6}$$

holds for the total energy balance with respect to an arbitrary reference configuration B and its boundary ∂B of (outer) orientation $\boldsymbol{n}$ (surface da and volume dv elements are left out of the notation for simplicity). Here,

$$f := \psi + k \tag{7}$$

is the sum of the free energy density ψ and kinetic energy density k, $\boldsymbol{f}$ represents the total energy flux density, s is the total supply rate density, and $\delta \geqslant 0$ is the dissipation rate density. For the current class of second-order continua with deformation microstructure, the basic constitutive forms

$$\begin{aligned} \boldsymbol{f} &= \boldsymbol{P}^{\mathrm{T}} \dot{\boldsymbol{\chi}} + \boldsymbol{P}^{\mathrm{T}} \nabla \dot{\boldsymbol{\chi}} + \boldsymbol{\Phi}^{\mathrm{T}} \dot{\boldsymbol{\varsigma}} - \sum_{a=1}^{m} \mu_a \boldsymbol{j}_a , \\ s &= \boldsymbol{b} \cdot \dot{\boldsymbol{\chi}} + \boldsymbol{\beta} \cdot \dot{\boldsymbol{\varsigma}} + \sum_{a=1}^{m} \mu_a \sigma_a , \\ \dot{k} &= \dot{\boldsymbol{m}} \cdot \dot{\boldsymbol{\chi}} + \dot{\boldsymbol{\mu}} \cdot \dot{\boldsymbol{\varsigma}} , \end{aligned} \tag{8}$$

hold for the energy flux, energy supply rate, and kinetic energy rate, densities, respectively. Here, $\boldsymbol{P}$ is the (first-order) first Piola-Kirchhoff stress, $\boldsymbol{P}$ is the corresponding second-order stress, $\boldsymbol{\Phi}$ represents the flux density associated with the evolution of $\boldsymbol{\varsigma}$, and $\mu_1, \dots, \mu_m$ represent the chemical potentials associated with $\varrho_1, \dots, \varrho_m$. The transpose $\boldsymbol{P}^{\mathrm{T}}$ of $\boldsymbol{P}$ is defined by $\boldsymbol{P}^{\mathrm{T}} \boldsymbol{A} \cdot \boldsymbol{a} := \boldsymbol{A} \cdot \boldsymbol{P} \boldsymbol{a}$. Note the symmetry $\boldsymbol{P} \cdot \boldsymbol{a} \otimes \boldsymbol{c} \otimes \boldsymbol{d} = \boldsymbol{P} \cdot \boldsymbol{a} \otimes \boldsymbol{d} \otimes \boldsymbol{c}$. Further, $\boldsymbol{m}$ is the standard momentum density, $\boldsymbol{b}$ represents the corresponding supply rate density, $\boldsymbol{\mu}$ is the microstructure momentum density, and $\boldsymbol{\beta}$ its supply rate density counterpart. In what follows, the notation $\boldsymbol{\mu} := (\mu_1, \dots, \mu_m)$ is also used for the array of chemical potentials; the context will make clear which is intended. In the context of Eqs. (7) and (8), localization of the energy balance equation (6) yields the form

$$\begin{aligned} \delta = {} & (\boldsymbol{P} + \operatorname{div} \boldsymbol{P}) \cdot \nabla \dot{\boldsymbol{\chi}} + \boldsymbol{P} \cdot \nabla \nabla \dot{\boldsymbol{\chi}} + \boldsymbol{\Phi} \cdot \nabla \dot{\boldsymbol{\varsigma}} \\ & + \sum_{a=1}^{m} \mu_a \dot{\varrho}_a - \boldsymbol{p} \cdot \dot{\boldsymbol{\chi}} - \boldsymbol{\pi} \cdot \dot{\boldsymbol{\varsigma}} - \dot{\psi} - \sum_{a=1}^{m} \boldsymbol{j}_a \cdot \nabla \mu_a \end{aligned} \tag{9}$$

for the dissipation rate density via Eq. (1), with

$$\begin{aligned} \boldsymbol{p} &:= \dot{\boldsymbol{m}} - \boldsymbol{b} - \operatorname{div} \boldsymbol{P} , \\ \boldsymbol{\pi} &:= \dot{\boldsymbol{\mu}} - \boldsymbol{\beta} - \operatorname{div} \boldsymbol{\Phi} , \end{aligned} \tag{10}$$

the production rate densities of standard and microstructural momentum, respectively. Given the above relations, we are now in a position to investigate the consequences of the Euclidean frame-indifference of the energy balance for the formulation, to which we now turn.

3 Euclidean frame-indifference of the energy balance

As usual, Euclidean frame-indifference of the energy balance is based on the transformation properties of the fields appearing in $\mathcal{E}$ from Eq. (6) with respect to change of Euclidean observer. These include f from Eq. (7), $\boldsymbol{f}$ and s from Eq. (8), and δ from Eq. (9). In fact, since δ as given by Eq. (9) follows directly from the localization of Eq. (6), the Euclidean frame-indifference of Eq. (6) is equivalent to that of δ as given by Eq. (9). As such, we examine the transformation properties of this latter field in what follows.

As usual (e.g., [1, §17], or [3, Chapter 6]), a change of Euclidean observer is represented via the corresponding time-dependent, spatially constant translation $\boldsymbol{c}$ and time-dependent, spatially constant orthogonal transformation $\boldsymbol{Q}$, such that

$$\boldsymbol{\chi}'(t,\boldsymbol{x}) = \boldsymbol{c}(t) + \boldsymbol{Q}(t)\,\boldsymbol{\chi}(t,\boldsymbol{x}) \tag{11}$$

follows for the transformation of the time-dependent deformation field $\boldsymbol{\chi}$ between an unprimed and primed observer. Since the results to follow must hold for any observer transformation, assume for simplicity that $\boldsymbol{Q}(0) = \boldsymbol{I}$ at the time origin $t = 0$. Then $\boldsymbol{\Omega} := \dot{\boldsymbol{Q}}(0)$ is skew-symmetric. Further, define $\boldsymbol{\omega} := \dot{\boldsymbol{c}}(0)$, $\varphi_0 := \varphi|_{t=0}$, and the deviation

$$[\![\varphi]\!] := (\varphi' - \boldsymbol{Q}_*\varphi)|_{t=0} \tag{12}$$

of some physical quantity φ from being Euclidean frame-indifferent (EFI). This latter is based on the action $\boldsymbol{Q}_*\varphi$ of $\boldsymbol{Q}$ on φ. For example, $\boldsymbol{Q}_*\boldsymbol{v} \equiv \boldsymbol{Q}\boldsymbol{v}$ in the case that $\varphi \equiv \boldsymbol{v}$ is spatially (i.e., as opposed to materially) vector-valued. In this context, the usual transformation relations

$$\begin{aligned}
&[\![\boldsymbol{\chi}]\!] = \boldsymbol{c}_0\,,\\
&[\![\nabla\boldsymbol{\chi}]\!] = \boldsymbol{0}\,,\quad [\![\nabla\nabla\boldsymbol{\chi}]\!] = \boldsymbol{0}\,,\\
&[\![\dot{\boldsymbol{\chi}}]\!] = \boldsymbol{\omega} + \boldsymbol{\Omega}\,\boldsymbol{\chi}_0\,,\quad [\![\nabla\dot{\boldsymbol{\chi}}]\!] = \boldsymbol{\Omega}\,\nabla\boldsymbol{\chi}_0\,,\\
&[\![\nabla\nabla\dot{\boldsymbol{\chi}}]\!] = \boldsymbol{\Omega}\,\nabla\nabla\boldsymbol{\chi}_0\,,
\end{aligned} \tag{13}$$

hold for $\boldsymbol{\chi}$ and its derivatives. Likewise, $\boldsymbol{\varsigma}$ is spatial and EFI. For this class of models, it suffices to restrict attention here to the case that $\boldsymbol{\varsigma}$ transforms as a spatial vector. This does not imply that $\boldsymbol{\varsigma}$ itself is vector-valued. For example, the deformation gradient $\boldsymbol{F} = \nabla\boldsymbol{\chi}$ transforms as a such a vector; this is also the case for the Cosserat or micropolar rotation and the micromorphic local deformation. Then $\boldsymbol{\varsigma}' = \boldsymbol{Q}_*\boldsymbol{\varsigma} \equiv \boldsymbol{Q}\boldsymbol{\varsigma}$ holds, implying

$$[\![\boldsymbol{\varsigma}]\!] = \boldsymbol{0},\quad [\![\nabla\boldsymbol{\varsigma}]\!] = \boldsymbol{0},\quad [\![\dot{\boldsymbol{\varsigma}}]\!] = \boldsymbol{\Omega}\,\boldsymbol{\varsigma}_0,\quad [\![\nabla\dot{\boldsymbol{\varsigma}}]\!] = \boldsymbol{\Omega}\,\nabla\boldsymbol{\varsigma}_0. \tag{14}$$

Note that all these are independent of $\boldsymbol{\omega}$.

Extending the result [3, Proposition 6.2.5] for the transformation between $\dot{\boldsymbol{m}}$ and $\boldsymbol{b}$ by analogy to $\dot{\boldsymbol{\mu}}$ and $\boldsymbol{\beta}$, we have

$$[\![\dot{\boldsymbol{m}}]\!] = [\![\boldsymbol{b}]\!] \quad\Longrightarrow\quad [\![\dot{\boldsymbol{\mu}}]\!] = [\![\boldsymbol{\beta}]\!]\,. \tag{15}$$

Further, the constitutive quantities $\dot{\psi}$, $\boldsymbol{P}$, P, $\boldsymbol{\Phi}$, μ_a and $\boldsymbol{j}_a$ are required to be EFI, in which case the restrictions

$$\begin{aligned}
&[\![\dot{\psi}]\!] = 0\,,\quad [\![\boldsymbol{P}]\!] = \boldsymbol{0}\,,\quad [\![\boldsymbol{\Phi}]\!] = \boldsymbol{0}\,,\\
&[\![P]\!] = \boldsymbol{0}\,,\quad [\![\mu_a]\!] = 0\,,\quad [\![\boldsymbol{j}_a]\!] = \boldsymbol{0}\,,
\end{aligned} \tag{16}$$

hold. On this basis,

$$\begin{aligned}
[\![\delta]\!] \;=\; &-\boldsymbol{p}_0\cdot\boldsymbol{\omega}\\
&+\{(\boldsymbol{P}+\operatorname{div}P)\,(\nabla\boldsymbol{\chi})^{\mathrm{T}}+P(\nabla\nabla\boldsymbol{\chi})^{\mathrm{T}}-\boldsymbol{p}\otimes\boldsymbol{\chi}\}_0\cdot\boldsymbol{\Omega}\\
&+\{\boldsymbol{\Phi}\,(\nabla\boldsymbol{\varsigma})^{\mathrm{T}}-\boldsymbol{\pi}\otimes\boldsymbol{\varsigma}\}_0\cdot\boldsymbol{\Omega}
\end{aligned} \tag{17}$$

follows for the transformation of δ from Eq. (9). Note that Eqs. (15) and $(16)_2$ imply $[\![\boldsymbol{p}]\!] = \boldsymbol{0}$ from Eq. $(10)_1$. The combination $\boldsymbol{P}\,(\nabla\boldsymbol{\chi})^{\mathrm{T}}$ is simply the usual (first-order) Kirchhoff stress. Analogously, we could interpret $P(\nabla\nabla\boldsymbol{\chi})^{\mathrm{T}}$ as a kind of second-order Kirchhoff stress. In any case, Eq. (17) must vanish as usual for arbitrary observer transformation for the energy balance to be EFI. As above, then, we are free to choose the simplest cases of (i) pure translation ($\boldsymbol{\Omega} = \boldsymbol{0}$), and (ii) pure orthogonal transformation ($\boldsymbol{\omega} = \boldsymbol{0}$). In particular, for a pure translation, Eq. (17) imply that $[\![\delta]\!]$ vanishes identically for arbitrary $\boldsymbol{\omega}$ iff $\boldsymbol{p}$ vanishes identically, i.e.,

$$\boldsymbol{p} = \boldsymbol{0} \quad\Longrightarrow\quad \dot{\boldsymbol{m}} = \operatorname{div}\boldsymbol{P} + \boldsymbol{b} \tag{18}$$

from Eq. $(10)_1$. In other words, $[\![\delta]\!]$ vanishes identically iff there is no momentum production, or alternatively, iff the standard momentum balance holds (e.g., [1,3,32]). Analogously, in case (ii), $[\![\delta]\!]$ vanishes identically iff

$$\begin{aligned}
&\operatorname{skw}\{(\boldsymbol{P}+\operatorname{div}P)\,(\nabla\boldsymbol{\chi})^{\mathrm{T}} + P(\nabla\nabla\boldsymbol{\chi})^{\mathrm{T}}\}\\
&\quad= \operatorname{skw}\{\boldsymbol{\pi}\otimes\boldsymbol{\varsigma} - \boldsymbol{\Phi}\,(\nabla\boldsymbol{\varsigma})^{\mathrm{T}}\}
\end{aligned} \tag{19}$$

holds. These represent direct generalizations of well-known results for first-order continua [1,19,20,32,38,68] to the current second-order case [1,21,22,36]. If we restrict attention to the classical forms

$$\boldsymbol{m} = \varrho\,\dot{\boldsymbol{\chi}}\,,\quad \boldsymbol{\mu} = \nu\,\dot{\boldsymbol{\varsigma}} \tag{20}$$

for the respective momentum densities based on constant referential mass density ϱ and microinertia ν, note that these results induce the better-known angular-momentum-based form

$$\dot{\boldsymbol{\Sigma}} = \operatorname{div} M + \operatorname{skw}\{(\nabla\boldsymbol{\chi})\,(\boldsymbol{P} + \operatorname{div} P)^{\mathrm{T}} + (\nabla\nabla\boldsymbol{\chi})\,P^{\mathrm{T}}\} + \boldsymbol{B} \tag{21}$$

of the microstructure balance equation $(10)_2$ via Eq. (19). Here,

$$\boldsymbol{\Sigma} := \operatorname{skw}\boldsymbol{\varsigma}\otimes\boldsymbol{\mu}, \quad M := \operatorname{skw}\boldsymbol{\varsigma}\otimes\boldsymbol{\Phi}, \quad \boldsymbol{B} := \operatorname{skw}\boldsymbol{\varsigma}\otimes\boldsymbol{\beta}, \tag{22}$$

represent the spin momentum density, corresponding flux density, and corresponding supply rate density, respectively. In these relations, the notation $(\operatorname{skw}\boldsymbol{\varsigma}\otimes\boldsymbol{\Phi})\,\boldsymbol{a} := \operatorname{skw}\boldsymbol{\varsigma}\otimes\boldsymbol{\Phi}\boldsymbol{a}$ has been used.

4 Free energy model

Again restricting attention to the case of elastic behavior with mass transfer, the constitutive form

$$\psi(\boldsymbol{\chi}, \nabla\boldsymbol{\chi}, \nabla\nabla\boldsymbol{\chi}, \boldsymbol{\varsigma}, \nabla\boldsymbol{\varsigma}, \varrho, \nabla\varrho, \boldsymbol{\phi}, \nabla\boldsymbol{\phi}) \tag{23}$$

for the (equilibrium) free energy density of the current constitutive class for second-order continua with microstructure. In particular, the dependence on gradients of the mass density and of the phase-field is the basic model expression of material heterogeneity in this context going back to Refs. [46] and [47] (see also Ref. [45]). From the more abstract viewpoint of material theory, the dependence ψ on ϱ, $\boldsymbol{\phi}$ and their gradients represents a model of material uniformity for ψ (e.g., [2,40]).

Being constitutive in nature, the form Eq. (23) of ψ for the current constitutive class is required to be material frame-indifferent [1], or equivalently, EFI and form-invariant [48, 49]. In this case, the restriction

$$\begin{aligned}&\psi(\boldsymbol{\chi}, \nabla\boldsymbol{\chi}, \nabla\nabla\boldsymbol{\chi}, \boldsymbol{\varsigma}, \nabla\boldsymbol{\varsigma}, \varrho, \nabla\varrho, \boldsymbol{\phi}, \nabla\boldsymbol{\phi})\\ &\quad = \psi(\boldsymbol{c} + \boldsymbol{Q}\boldsymbol{\chi}, \boldsymbol{Q}\nabla\boldsymbol{\chi}, \boldsymbol{Q}\nabla\nabla\boldsymbol{\chi}, \boldsymbol{Q}\boldsymbol{\varsigma}, \boldsymbol{Q}\nabla\boldsymbol{\varsigma}, \varrho, \nabla\varrho, \boldsymbol{\phi}, \nabla\boldsymbol{\phi})\end{aligned} \tag{24}$$

on the form of ψ holds for all translations $\boldsymbol{c}$ and all orthogonal transformations $\boldsymbol{Q}$. For fixed arguments $\boldsymbol{\chi}, \boldsymbol{\varsigma}, \nabla\boldsymbol{\chi}, \nabla\boldsymbol{\varsigma}, \nabla\nabla\boldsymbol{\chi}$, $\varrho, \nabla\varrho, \boldsymbol{\phi}, \nabla\boldsymbol{\phi}$, the left-hand side of Eq. (24) is constant. As such, the time-derivative of Eq. $(24)_1$ at $t = 0$ yields the result

$$\begin{aligned}0 \;&= \{\partial_{\boldsymbol{\chi}}\psi\}_0 \cdot \boldsymbol{\omega}\\ &\quad + \{\partial_{\boldsymbol{\chi}}\psi\otimes\boldsymbol{\chi} + \partial_{\nabla\boldsymbol{\chi}}\psi\,(\nabla\boldsymbol{\chi})^{\mathrm{T}} + \partial_{\nabla\nabla\boldsymbol{\chi}}\psi\,(\nabla\nabla\boldsymbol{\chi})^{\mathrm{T}}\}_0 \cdot \boldsymbol{\Omega}\\ &\quad + \{\partial_{\boldsymbol{\varsigma}}\psi\otimes\boldsymbol{\varsigma} + \partial_{\nabla\boldsymbol{\varsigma}}\psi\,(\nabla\boldsymbol{\varsigma})^{\mathrm{T}}\}_0 \cdot \boldsymbol{\Omega}\end{aligned} \tag{25}$$

for the case that $\boldsymbol{\varsigma}$ is spatial. Then $[\![\dot{\psi}]\!] = 0$ follows, as assumed in Eq. $(16)_1$. Since Eq. (25) holds for arbitrary observer transformations, we are free to choose the simplest cases of (i) pure translation ($\boldsymbol{\Omega} = \boldsymbol{0}$), and (ii) pure orthogonal transformation ($\boldsymbol{\omega} = \boldsymbol{0}$). In case (i), $\partial_{\boldsymbol{\chi}}\psi = \boldsymbol{0}$ holds identically since $\boldsymbol{c}$ and the time origin $t = 0$ are arbitrary. This reduces Eq. (23) to

$$\psi = \psi(\nabla\boldsymbol{\chi}, \nabla\nabla\boldsymbol{\chi}, \boldsymbol{\varsigma}, \nabla\boldsymbol{\varsigma}, \varrho, \nabla\varrho, \boldsymbol{\phi}, \nabla\boldsymbol{\phi}) \tag{26}$$

independent of $\boldsymbol{\chi}$ as expected. Analogously, in case (ii), Eq. (25) holds identically, i.e., for arbitrary $\boldsymbol{\Omega}$ and time origin $t = 0$, iff

$$\begin{aligned}&\operatorname{skw}\{\partial_{\nabla\boldsymbol{\chi}}\psi\,(\nabla\boldsymbol{\chi})^{\mathrm{T}} + \partial_{\nabla\nabla\boldsymbol{\chi}}\psi\,(\nabla\nabla\boldsymbol{\chi})^{\mathrm{T}}\}\\ &\quad = -\operatorname{skw}\{\partial_{\boldsymbol{\varsigma}}\psi\otimes\boldsymbol{\varsigma} + \partial_{\nabla\boldsymbol{\varsigma}}\psi\,(\nabla\boldsymbol{\varsigma})^{\mathrm{T}}\}\end{aligned} \tag{27}$$

holds. As in case (i), these represent restrictions on the functional form Eq. (26) of ψ. Note the formal similarity of these restrictions to those of Eq. (19) based on the Euclidean frame-indifference of δ and the energy balance. As discussed below, they in fact converge in the current case of gradient hyperelasticity.

5 Dissipation principle

With the basic results and restrictions Eqs. (18), (19), and (26) in hand, we now return to the thermodynamic formulation. Substitution of these into the expression (9) for the dissipation rate density and integration over B yields

$$\begin{aligned}\int_B \delta \;&= \int_B (\boldsymbol{P} + \operatorname{div} P - \partial_{\nabla\boldsymbol{\chi}}\psi)\cdot\nabla\dot{\boldsymbol{\chi}} + (P - \partial_{\nabla\nabla\boldsymbol{\chi}}\psi)\cdot\nabla\nabla\dot{\boldsymbol{\chi}}\\ &\quad + \int_B (\boldsymbol{\Phi} - \partial_{\nabla\boldsymbol{\varsigma}}\psi)\cdot\nabla\dot{\boldsymbol{\varsigma}} - (\boldsymbol{\pi} + \partial_{\boldsymbol{\varsigma}}\psi)\cdot\dot{\boldsymbol{\varsigma}}\\ &\quad + \sum_{a=1}^{m}\int_B (\mu_a - \delta_{\varrho_a}\psi)\,\dot{\varrho}_a - \boldsymbol{j}_a\cdot\nabla\mu_a - \sum_{\alpha=1}^{p}\int_B \delta_{\phi_\alpha}\psi\,\dot{\phi}_\alpha\\ &\quad - \sum_{a=1}^{m}\int_{\partial B}\partial_{\nabla\varrho_a}\psi\cdot\boldsymbol{n}\,\dot{\varrho}_a - \sum_{\alpha=1}^{p}\int_{\partial B}\partial_{\nabla\phi_\alpha}\psi\cdot\boldsymbol{n}\,\dot{\phi}_\alpha\end{aligned} \tag{28}$$

for the dissipation rate with respect to B via integration by parts and the divergence theorem. The variational derivative

$$\delta_x\psi = \partial_x\psi - \operatorname{div}\partial_{\nabla x}\psi \tag{29}$$

appears here because the system is materially inhomogeneous. Modeling P, $\boldsymbol{\Phi}$, $\boldsymbol{\pi}$, μ_a and $\boldsymbol{P}$ as purely energetic, Eq. (28) implies

$$P = \partial_{\nabla\nabla\boldsymbol{\chi}}\psi\,, \quad \boldsymbol{\pi} = -\partial_{\boldsymbol{\varsigma}}\psi\,, \quad \boldsymbol{\Phi} = \partial_{\nabla\boldsymbol{\varsigma}}\psi\,, \quad \mu_a = \delta_{\varrho_a}\psi\,, \tag{30}$$

and

$$\boldsymbol{P} = \partial_{\nabla \chi} \psi - \operatorname{div} \boldsymbol{P} = \partial_{\nabla \chi} \psi - \operatorname{div} \partial_{\nabla \nabla \chi} \psi = \delta_{\nabla \chi} \psi \,. \quad (31)$$

On the basis of Eqs. (30) and (31), note in particular that the EFI-based result (19) for moment of momentum balance reduces to the restriction (27) on ψ from material frame-indifference. This presents a generalization to gradient continua and continua with microstructure of the old result of Noll [50] that the material frame-indifference of the "strain energy" is necessary and sufficient for the symmetry of the Cauchy stress and so for moment of momentum balance.

Given Eqs. (30) and (31), Eq. (28) reduces to

$$\begin{aligned} \int_B \delta \;=\; & -\sum_{a=1}^{m} \int_B \boldsymbol{j}_a \cdot \nabla \mu_a - \sum_{\alpha=1}^{p} \int_B \delta_{\phi_\alpha} \psi \, \dot{\phi}_\alpha \\ & - \sum_{a=1}^{m} \int_{\partial B} \partial_{\nabla \varrho_a} \psi \cdot \boldsymbol{n} \, \dot{\varrho}_a - \sum_{\alpha=1}^{p} \int_{\partial B} \partial_{\nabla \phi_\alpha} \psi \cdot \boldsymbol{n} \, \dot{\phi}_\alpha \end{aligned} \quad (32)$$

for the dissipation rate with respect to B. As evident, the boundary terms appearing in Eq. (32) represent boundary-based contributions to the dissipation rate in the material. Clearly, these terms vanish identically in the case of no-flux boundary conditions

$$\partial_{\nabla \varrho_a} \psi \cdot \boldsymbol{n} = 0 \,, \quad \partial_{\nabla \phi_\alpha} \psi \cdot \boldsymbol{n} = 0 \,, \quad (33)$$

on (the flux part of) ∂B. This is also the case for time-independent Dirichlet boundary conditions

$$\dot{\varrho}_a = 0 \,, \quad \dot{\phi}_\alpha = 0 \,, \quad (34)$$

on (the rate part of) ∂B. Both of these possibilities can be expressed in the combined form

$$\partial_{\nabla \varrho_a} \psi \cdot \boldsymbol{n} \, \dot{\varrho}_a = 0 \,, \quad \partial_{\nabla \phi_\alpha} \psi \cdot \boldsymbol{n} \, \dot{\phi}_\alpha = 0 \,, \quad (35)$$

on ∂B for each constituent a and each phase α. These include in particular no-flux boundary conditions with respect to the mass density and phase fields. In any case, boundary conditions are part of the physical model formulation. From a material theoretic point of view, boundary conditions have the same character as constitutive relations in the case of materially heterogeneous systems. In any case, these result in the reduced or "residual" form

$$\delta = -\sum_{a=1}^{m} \boldsymbol{j}_a \cdot \nabla \mu_a - \sum_{\alpha=1}^{p} \dot{\phi}_\alpha \, \delta_{\phi_\alpha} \psi \quad (36)$$

for the dissipation-rate density δ from Eq. (32).

As is well-known, in the context of non-equilibrium thermodynamics and transport theory (e.g., [3,51,52]), the form Eq. (36) of the residual dissipation-rate density δ forms the basis of dissipative-kinetic thermodynamic "flux-force" relations. As usual, from a physical point of view, spatial gradients like $-\nabla \mu_a$ are interpreted as "forces" in the sense that each drives a corresponding (spatial) flux like $\boldsymbol{j}_a$ resulting in non-negative dissipation. Analogously, $-\delta_{\phi_\alpha} \psi$ drives the (temporal) "flux" $\dot{\phi}_\alpha$ resulting in non-negative dissipation. Let

$$\begin{aligned} \boldsymbol{j} &:= (\boldsymbol{j}_1, \dots, \boldsymbol{j}_m, \dot{\phi}_1, \dots, \dot{\phi}_p) \,, \\ \boldsymbol{f} &:= -(\nabla \mu_1, \dots, \nabla \mu_m, \delta_{\phi_1} \psi, \dots, \delta_{\phi_p} \psi) \,. \end{aligned} \quad (37)$$

In general, the fluxes $\boldsymbol{j}$ are assumed to depend constitutively on driving forces $\boldsymbol{f}$, i.e., $\boldsymbol{j}(\boldsymbol{f})$. In particular, $\boldsymbol{j}(\boldsymbol{0}) = \boldsymbol{0}$. Assuming that $\boldsymbol{j}(\boldsymbol{f})$ is smooth (analytic), note that its Taylor-series expansion

$$\boldsymbol{j}(\boldsymbol{f}) = \partial_{\boldsymbol{f}} \boldsymbol{j}(\boldsymbol{0}) \, \boldsymbol{f} + \frac{1}{2} \left(\partial_{\boldsymbol{f}} \partial_{\boldsymbol{f}} \boldsymbol{j}(\boldsymbol{0}) \, \boldsymbol{f} \right) \boldsymbol{f} + \cdots \quad (38)$$

about $\boldsymbol{f} = \boldsymbol{0}$ assuming $\boldsymbol{j}(\boldsymbol{0}) = \boldsymbol{0}$ can be expressed in quasi-linear form11

$$\boldsymbol{j}(\boldsymbol{f}) = \left\{ \partial_{\boldsymbol{f}} \boldsymbol{j}(\boldsymbol{0}) + \frac{1}{2} \, \partial_{\boldsymbol{f}} \partial_{\boldsymbol{f}} \boldsymbol{j}(\boldsymbol{0}) \, \boldsymbol{f} + \cdots \right\} \boldsymbol{f} =: \boldsymbol{L}(\boldsymbol{f}) \, \boldsymbol{f} \,, \quad (39)$$

depending on the (generalized) "matrix" $\boldsymbol{L}$ of transport "coefficients". In these terms, the (in)famous bilinear form

$$\delta = \boldsymbol{j} \cdot \boldsymbol{f} = \boldsymbol{f} \cdot \boldsymbol{j} = \boldsymbol{f} \cdot \boldsymbol{L} \boldsymbol{f} \quad (40)$$

follows for the residual dissipation rate density δ from Eq. (36). This last result implies that only the symmetric part of $\boldsymbol{L}$ contributes to δ (c.f. [53]). As usual, modeling $\boldsymbol{L}$ as non-negative definite is sufficient to satisfy $\delta \geqslant 0$, i.e., $\boldsymbol{f} \cdot \boldsymbol{L} \boldsymbol{f} \geqslant 0$ for all $\boldsymbol{f}$.

A special case of the quasi-linear form Eq. (39) is a potential form for $\boldsymbol{j}(\boldsymbol{f})$; in the context of Eq. (39), the conditions for the existence of a potential representation for $\boldsymbol{j}(\boldsymbol{f})$ are contingent on $\boldsymbol{L}(\boldsymbol{f})$ satisfying additional constraints (e.g., related to integrability). These have been examined in detail for in Ref. [53]. For the purpose of the current model formulation and in particular that of the corresponding IBVP, it will be assumed for simplicity that these are satisfied identically. In this case, the potential forms

$$\boldsymbol{j}_a = -\partial_{\nabla \mu_a} \boldsymbol{\chi} \,, \quad \dot{\phi}_\alpha = -\partial_{\delta_{\phi_\alpha} \psi} \boldsymbol{\chi} \,, \quad (41)$$

of Eq. (39) hold in terms of a dissipation potential

$$\boldsymbol{\chi}(\dots, \nabla \mu_1, \dots, \nabla \mu_m, \delta_{\phi_1} \psi, \dots, \delta_{\phi_p} \psi) \,. \quad (42)$$

In this case,

$$\delta = \sum_{a=1}^{m} \nabla\mu_a \cdot \partial_{\nabla\mu_a} \boldsymbol{\chi} + \sum_{\alpha=1}^{p} \delta_{\phi_\alpha}\psi \; \partial_{\delta_{\phi_\alpha}\psi} \boldsymbol{\chi} \tag{43}$$

follows for δ from Eq. (36). Sufficient to fulfill the dissipation principle $\delta \geqslant 0$ is the modeling of $\boldsymbol{\chi}$ as non-negative $\chi \geqslant 0$ and convex

$$\sum_{a=1}^{m} \nabla\mu_a \cdot \partial_{\nabla\mu_a} \chi + \sum_{\alpha=1}^{p} \delta_{\phi_\alpha}\psi \; \partial_{\delta_{\phi_\alpha}\psi} \chi \geqslant \chi \,, \tag{44}$$

in the forces. In this case, $\delta \geqslant \chi \geqslant 0$ from Eq. (43), sufficient for fulfillment of the dissipation principle (e.g., [3, Chapter9]) or non-negative entropy production.

6 Rate variational form of reduced field relations

Combining Eqs. (1), $(30)_4$ and $(41)_1$ results in the coupled system

$$\delta_{\varrho_a}\psi = \mu_a \,, \quad \dot{\varrho}_a = \operatorname{div} \partial_{\nabla\mu_a}\chi + \sigma_a \,, \tag{45}$$

of field relations for the pair (ϱ_a, μ_a). In the simplest case, $\sigma_a = 0$ and χ from Eq. (42) is quadratic in $\nabla\mu_a$. In this case, these last two relations combine to yield the Cahn–Hilliard equation

$$\dot{\varrho}_a = \operatorname{div} m_a \nabla \delta_{\varrho_a}\psi \tag{46}$$

for ϱ_a in terms of the chemical mobility m_a. Again, in the simplest case, χ is also quadratic in $\delta_{\phi_\alpha}\psi$, in which case Eq. $(41)_2$ reduces to

$$\dot{\phi}_\alpha = -m_\alpha \, \delta_{\phi_\alpha}\psi \,, \tag{47}$$

representing the time-dependent Ginzburg–Landau equation for ϕ_α in terms of the corresponding relaxational mobility m_α. To these we add the standard linear

$$\dot{\boldsymbol{m}} = \operatorname{div} \delta_{\nabla\boldsymbol{\chi}}\psi + \boldsymbol{b} = -\delta^2_{\boldsymbol{\chi}}\psi + \boldsymbol{b} \tag{48}$$

and microstructure

$$\dot{\boldsymbol{\mu}} = -\partial_{\boldsymbol{\varsigma}}\psi + \operatorname{div} \partial_{\nabla\boldsymbol{\varsigma}}\psi + \boldsymbol{\beta} = -\delta_{\boldsymbol{\varsigma}}\psi + \boldsymbol{\beta} \tag{49}$$

momentum balances from Eqs. (10), (18), (30) and (31) in terms of the first-order Eq. (29) and second-order

$$\delta^2_x\psi := \partial_x\psi - \operatorname{div} \partial_{\nabla x}\psi + \operatorname{div}\operatorname{div} \partial_{\nabla\nabla x}\psi \tag{50}$$

variational derivatives.

A unified variational formulation of the reduced field relations and boundary conditions can be obtained as follows [39,41]. To this end, note that Eqs. (30), (31) and $(41)_1$ imply

$$\begin{aligned} \dot{\varrho}_a + \operatorname{div} \boldsymbol{j}_a &= \delta_{\mu_a} r_{\mathrm{i}} \,, \\ \dot{\boldsymbol{m}} - \boldsymbol{p} - \operatorname{div} \boldsymbol{P} &= \delta^2_{\boldsymbol{\chi}} r_{\mathrm{i}} \,, \\ \dot{\boldsymbol{\mu}} - \boldsymbol{\pi} - \operatorname{div} \boldsymbol{\Phi} &= \delta_{\boldsymbol{\varsigma}} r_{\mathrm{i}} \,, \end{aligned} \tag{51}$$

in terms of the (internal) rate potential density

$$r_{\mathrm{i}} := \dot{f} - \sum_{a=1}^{m} \mu_a \, \dot{\varrho}_a + d = \dot{\psi} - \boldsymbol{\mu} \cdot \dot{\boldsymbol{\varrho}} + \dot{k} + d \tag{52}$$

based on the dynamic energy storage rate density

$$\begin{aligned} \dot{f} \; &= \dot{\boldsymbol{m}} \cdot \dot{\boldsymbol{\chi}} + \partial_{\nabla\boldsymbol{\chi}}\psi \cdot \nabla\dot{\boldsymbol{\chi}} + \partial_{\nabla\nabla\boldsymbol{\chi}}\psi \cdot \nabla\nabla\dot{\boldsymbol{\chi}} \\ &\quad + (\dot{\boldsymbol{\mu}} + \partial_{\boldsymbol{\varsigma}}\psi) \cdot \dot{\boldsymbol{\varsigma}} + \partial_{\nabla\boldsymbol{\varsigma}}\psi \cdot \nabla\dot{\boldsymbol{\varsigma}} \\ &\quad + \partial_{\boldsymbol{\varrho}}\psi \cdot \dot{\boldsymbol{\varrho}} + \partial_{\nabla\boldsymbol{\varrho}}\psi \cdot \nabla\dot{\boldsymbol{\varrho}} + \partial_{\boldsymbol{\phi}}\psi \cdot \dot{\boldsymbol{\phi}} + \partial_{\nabla\boldsymbol{\phi}}\psi \cdot \nabla\dot{\boldsymbol{\phi}} \end{aligned} \tag{53}$$

from Eqs. (7), $(8)_3$ and (26) as well as the dual form

$$d(\ldots, \nabla\boldsymbol{\mu}, \dot{\boldsymbol{\phi}}) \tag{54}$$

of the dissipation potential χ from Eq. (54) concave in $\nabla\boldsymbol{\mu}$ and convex in $\dot{\boldsymbol{\phi}}$. Given Eq. (51), the compact forms

$$\delta_{\boldsymbol{\mu}} r_{\mathrm{i}} = -\boldsymbol{\sigma} \,, \quad \delta^2_{\dot{\boldsymbol{\chi}}} r_{\mathrm{i}} = \boldsymbol{b} \,, \quad \delta_{\dot{\boldsymbol{\varsigma}}} r_{\mathrm{i}} = \boldsymbol{\beta} \,, \tag{55}$$

for Eqs. (1), (18) and $(10)_2$ follow in terms of the corresponding variational derivatives of r_{i}. The analogous relations

$$\delta_{\dot{\boldsymbol{\varrho}}} r_{\mathrm{i}} = \boldsymbol{0} \,, \quad \delta_{\dot{\boldsymbol{\phi}}} r_{\mathrm{i}} = \boldsymbol{0} \,, \tag{56}$$

are obtained from Eqs. $(30)_4$ and $(41)_2$, respectively. Given the variational form Eqs. (55) and (56) of the basic balance and field relations of the current formulation, we are in a position to formulate the corresponding IBVP in variational form, our next task.

7 Rate variational formulation of the IBVP

As has been recognized and exploited in earlier work [39,41,42], and as attested to by the current results Eqs. (55) and (56), the physical modeling of energetic and kinetic effects as based on corresponding potentials Eqs. (26) and (54), respectively, facilitates a rate variational formulation of the corresponding IBVP. In the current case, the "rates" involved are $\dot{\boldsymbol{\varrho}}$, $\boldsymbol{\mu}$, $\dot{\boldsymbol{\chi}}$, $\dot{\boldsymbol{\varsigma}}$, $\dot{\boldsymbol{\phi}}$.

To be consistent with the formulation up to this point, the no-flux boundary conditions equation (33) are assumed. To these we add the no mass flux condition

$$\boldsymbol{j}_a \cdot \boldsymbol{n} = \partial_{\nabla \mu_a} r_{\mathrm{i}} \cdot \boldsymbol{n} = 0\,,\ a = 1, \ldots, m\,, \tag{57}$$

on ∂B. Turning next to the kinematic fields, for simplicity, attention is restricted to loading environments of the rate-flux (e.g., generalized displacement-traction) type (e.g., [3]) here; other such conditions (e.g., unilateral or bilateral generalized contact) are possible. By analogy with the case of the deformation or displacement gradient in the context of elasticity [22,36], $\dot{\boldsymbol{\chi}}$ and $\nabla\dot{\boldsymbol{\chi}}$, as well as their variations, are not necessarily independent on ∂B. Indeed, by analogy with the flux itself, only the normal part $\nabla_{\boldsymbol{n}}\,\delta\dot{\boldsymbol{\chi}} = (\nabla\dot{\boldsymbol{\chi}})\,\boldsymbol{n}$ can be considered so. Consequently, consider the split

$$\nabla\dot{\boldsymbol{\chi}} = \nabla_{\boldsymbol{n}}\,\dot{\boldsymbol{\chi}} \otimes \boldsymbol{n} + \nabla_{\mathrm{s}}\,\dot{\boldsymbol{\chi}} \tag{58}$$

of $\nabla\dot{\boldsymbol{\chi}}$ on ∂B into normal $\nabla_{\boldsymbol{n}}\,\dot{\boldsymbol{\chi}} = (\nabla\dot{\boldsymbol{\chi}})\,\boldsymbol{n}$ and tangential or in-surface $\nabla_{\mathrm{s}}\,\dot{\boldsymbol{\chi}}$ parts, respectively. On this basis, the independent kinematic fields on ∂B are $\dot{\boldsymbol{\chi}}$, $\nabla_{\boldsymbol{n}}\,\dot{\boldsymbol{\chi}}$, and $\dot{\boldsymbol{\varsigma}}$. The thermodynamically conjugate boundary normal flux densities are $\boldsymbol{t}$, $\boldsymbol{s}$, and $\boldsymbol{\varphi}$, respectively. These determine the total boundary normal energy flux density on the flux part of ∂B via

$$\boldsymbol{f} \cdot \boldsymbol{n} = \boldsymbol{t} \cdot \dot{\boldsymbol{\chi}} + \boldsymbol{s} \cdot \nabla_{\boldsymbol{n}}\,\dot{\boldsymbol{\chi}} + \boldsymbol{\varphi} \cdot \dot{\boldsymbol{\varsigma}} \tag{59}$$

from Eq. $(8)_1$ on (the flux part of) ∂B.

The variational formulation of the energy supply rate density Eq. $(8)_2$, supply rate densities in Eq. (55), and boundary energy flux density (59) consistent with the above boundary conditions, is based on rate potential densities r_{s} and r_{f}, respectively, analogous to r_{i}. In terms of these, we have

$$\begin{aligned} \boldsymbol{f} \cdot \boldsymbol{n} &= -\partial_{\dot{\boldsymbol{\chi}}} r_{\mathrm{f}} \cdot \dot{\boldsymbol{\chi}} - \partial_{\nabla_{\boldsymbol{n}}\dot{\boldsymbol{\chi}}} r_{\mathrm{f}} \cdot \nabla_{\boldsymbol{n}}\,\dot{\boldsymbol{\chi}} - \partial_{\dot{\boldsymbol{\varsigma}}} r_{\mathrm{f}} \cdot \dot{\boldsymbol{\varsigma}}\,, \\ s &= -\partial_{\dot{\boldsymbol{\chi}}} r_{\mathrm{s}} \cdot \dot{\boldsymbol{\chi}} - \partial_{\dot{\boldsymbol{\varsigma}}} r_{\mathrm{s}} \cdot \dot{\boldsymbol{\varsigma}} + \partial_{\boldsymbol{\mu}} r_{\mathrm{s}} \cdot \boldsymbol{\mu}\,, \end{aligned} \tag{60}$$

via

$$\boldsymbol{t} = -\partial_{\dot{\boldsymbol{\chi}}} r_{\mathrm{f}}\,, \quad \boldsymbol{s} = -\partial_{\nabla_{\boldsymbol{n}}\dot{\boldsymbol{\chi}}} r_{\mathrm{f}}\,, \quad \boldsymbol{\varphi} = -\partial_{\dot{\boldsymbol{\varsigma}}} r_{\mathrm{f}}\,, \tag{61}$$

and

$$\boldsymbol{b} = -\partial_{\dot{\boldsymbol{\chi}}} r_{\mathrm{s}}\,, \quad \boldsymbol{\beta} = -\partial_{\dot{\boldsymbol{\varsigma}}} r_{\mathrm{s}}\,, \quad \boldsymbol{\sigma} = \partial_{\boldsymbol{\mu}} r_{\mathrm{s}}\,. \tag{62}$$

Introducing then the combined rate potential density

$$r_{\mathrm{v}} := r_{\mathrm{i}} + r_{\mathrm{s}}\,, \tag{63}$$

Eq. (55) reduce to

$$\delta_{\boldsymbol{\mu}} r_{\mathrm{v}} = \boldsymbol{0}\,, \quad \delta^2_{\dot{\boldsymbol{\chi}}} r_{\mathrm{v}} = \boldsymbol{0}\,, \quad \delta_{\dot{\boldsymbol{\varsigma}}} r_{\mathrm{v}} = \boldsymbol{0}\,. \tag{64}$$

Together with Eq. (56), these form the basis of the variational formulation of the IBVP for the current case of second-order continua with microstructure (e.g. [39,41]). To this end, one works with the rate functional

$$\mathcal{R} = \mathcal{R}_B + \mathcal{R}_{\partial B} = \int_B r_{\mathrm{v}} + \int_{\partial B} r_{\mathrm{f}}\,. \tag{65}$$

To see this, consider the first variations

$$\begin{aligned} \delta\mathcal{R}_B \ &= \int_B \partial_{\dot{\boldsymbol{\chi}}} r_{\mathrm{v}} \cdot \delta\dot{\boldsymbol{\chi}} + \partial_{\nabla\dot{\boldsymbol{\chi}}} r_{\mathrm{v}} \cdot \delta\nabla\dot{\boldsymbol{\chi}} + \partial_{\nabla\nabla\dot{\boldsymbol{\chi}}} r_{\mathrm{v}} \cdot \delta\nabla\nabla\dot{\boldsymbol{\chi}} \\ &\quad + \int_B \partial_{\dot{\boldsymbol{\varsigma}}} r_{\mathrm{v}} \cdot \delta\dot{\boldsymbol{\varsigma}} + \partial_{\nabla\dot{\boldsymbol{\varsigma}}} r_{\mathrm{v}} \cdot \delta\nabla\dot{\boldsymbol{\varsigma}} \\ &\quad + \int_B \partial_{\boldsymbol{x}} r_{\mathrm{v}} \cdot \delta\boldsymbol{x} + \partial_{\nabla\boldsymbol{x}} r_{\mathrm{v}} \cdot \delta\nabla\boldsymbol{x} \end{aligned} \tag{66}$$

with $\boldsymbol{x} := (\dot{\boldsymbol{\varrho}}, \boldsymbol{\mu}, \dot{\boldsymbol{\phi}})$ and

$$\delta\mathcal{R}_{\partial B} = \int_{\partial B} \partial_{\dot{\boldsymbol{\chi}}} r_{\mathrm{f}} \cdot \delta\dot{\boldsymbol{\chi}} + \partial_{\nabla_{\boldsymbol{n}}\dot{\boldsymbol{\chi}}} r_{\mathrm{f}} \cdot \delta\nabla_{\boldsymbol{n}}\,\dot{\boldsymbol{\chi}} + \partial_{\dot{\boldsymbol{\varsigma}}} r_{\mathrm{f}} \cdot \delta\dot{\boldsymbol{\varsigma}} \tag{67}$$

in the rates, with

$$\delta_{\nabla_{\boldsymbol{n}}\dot{\boldsymbol{\chi}}} r := (\delta_{\nabla\dot{\boldsymbol{\chi}}} r)\,\boldsymbol{n}\,, \qquad \partial_{\nabla_{\boldsymbol{n}}\nabla_{\boldsymbol{n}}\dot{\boldsymbol{\chi}}} r := (\partial_{\nabla\nabla\dot{\boldsymbol{\chi}}} r)\,\boldsymbol{n} \otimes \boldsymbol{n}\,, \tag{68}$$

and analogously for $\partial_{\nabla_{\boldsymbol{n}}\dot{\boldsymbol{\varsigma}}} r$. Via repeated application of integration by parts and the divergence theorem, combination of $\delta\mathcal{R}_B$ and $\delta\mathcal{R}_{\partial B}$ then yield

$$\begin{aligned} \delta\mathcal{R} = &\int_B \delta^2_{\dot{\boldsymbol{\chi}}} r_{\mathrm{v}} \cdot \delta\dot{\boldsymbol{\chi}} + \delta_{\dot{\boldsymbol{\varsigma}}} r_{\mathrm{v}} \cdot \delta\dot{\boldsymbol{\varsigma}} + \delta_{\boldsymbol{x}} r_{\mathrm{v}} \cdot \delta\boldsymbol{x} \\ &+ \int_{\partial B} \{\partial_{\dot{\boldsymbol{\chi}}} r_{\mathrm{f}} + \delta_{\nabla_{\boldsymbol{n}}\dot{\boldsymbol{\chi}}} r_{\mathrm{v}} + \kappa_{\mathrm{s}}\,\partial_{\nabla_{\boldsymbol{n}}\nabla_{\boldsymbol{n}}\dot{\boldsymbol{\chi}}} r_{\mathrm{v}} \\ &- \mathrm{div}_{\mathrm{s}}\,\partial_{\nabla_{\boldsymbol{n}}\nabla\dot{\boldsymbol{\chi}}} r_{\mathrm{v}}\} \cdot \delta\dot{\boldsymbol{\chi}} \\ &+ \int_{\partial B} \{\partial_{\nabla_{\boldsymbol{n}}\dot{\boldsymbol{\chi}}} r_{\mathrm{f}} + \partial_{\nabla_{\boldsymbol{n}}\nabla_{\boldsymbol{n}}\dot{\boldsymbol{\chi}}} r_{\mathrm{v}}\} \cdot \delta\nabla_{\boldsymbol{n}}\,\dot{\boldsymbol{\chi}} \\ &+ \int_{\partial B} \{\partial_{\dot{\boldsymbol{\varsigma}}} r_{\mathrm{f}} + \partial_{\nabla_{\boldsymbol{n}}\dot{\boldsymbol{\varsigma}}} r_{\mathrm{v}}\} \cdot \delta\dot{\boldsymbol{\varsigma}} \\ &+ \int_{\partial B} \partial_{\nabla_{\boldsymbol{n}}\boldsymbol{x}} r_{\mathrm{v}} \cdot \delta\boldsymbol{x} \end{aligned} \tag{69}$$

for the first variation $\delta\mathcal{R}$ of R, with $\kappa_{\mathrm{s}} := \mathrm{div}_{\mathrm{s}}\,\boldsymbol{n}$. On this basis, the corresponding stationarity conditions are then

$$\delta^2_{\dot{\boldsymbol{\chi}}} r_{\mathrm{v}} = \boldsymbol{0}\,, \quad \delta_{\dot{\boldsymbol{\varsigma}}} r_{\mathrm{v}} = \boldsymbol{0}\,, \quad \delta_{\boldsymbol{x}} r_{\mathrm{v}} = \boldsymbol{0}\,, \tag{70}$$

in B corresponding to Eqs. (56) and (64), as well as

$$\begin{aligned} \boldsymbol{0} &= \partial_{\dot{\boldsymbol{\chi}}} r_{\mathrm{f}} + \delta_{\nabla_{\boldsymbol{n}}\dot{\boldsymbol{\chi}}} r_{\mathrm{v}} + \kappa_{\mathrm{s}}\,\partial_{\nabla_{\boldsymbol{n}}\nabla_{\boldsymbol{n}}\dot{\boldsymbol{\chi}}} r_{\mathrm{v}} - \mathrm{div}_{\mathrm{s}}\,\partial_{\nabla_{\boldsymbol{n}}\nabla\dot{\boldsymbol{\chi}}} r_{\mathrm{v}}\,, \\ \boldsymbol{0} &= \partial_{\nabla_{\boldsymbol{n}}\dot{\boldsymbol{\chi}}} r_{\mathrm{f}} + \partial_{\nabla_{\boldsymbol{n}}\nabla_{\boldsymbol{n}}\dot{\boldsymbol{\chi}}} r_{\mathrm{v}}\,, \\ \boldsymbol{0} &= \partial_{\dot{\boldsymbol{\varsigma}}} r_{\mathrm{f}} + \partial_{\nabla_{\boldsymbol{n}}\dot{\boldsymbol{\varsigma}}} r_{\mathrm{v}}\,, \\ \boldsymbol{0} &= \partial_{\nabla_{\boldsymbol{n}}\boldsymbol{x}} r_{\mathrm{v}}\,, \end{aligned} \tag{71}$$

on ∂B in agreement with Eqs. (33), (57) and (61).

As discussed in more detail in Refs. [39,41], this results in bounds on the energy balance as well. Along with the variational formulation itself, such bounds provide the basis

for stability and other considerations which are the focus of current research on such continua.

8 Discussion

As witnessed by the vast literature on the subject, the continuum thermodynamic and rate variational approach utilized in this work is but one among many which has been employed to formulate phenomenological "mean-field" models for generalized continua with microstructure. As hinted at in the introduction, there are at least two approaches in this regard in the literature. From a conceptual point of view, at least, each of these approaches is quite different in character.

In a nutshell, the first approach postulates a variational or variational-like principle from the start. A classic example of this is a space-time action principle (e.g., [23,36]). More recent are formulations based on variational-like principles of pure mechanics such as virtual work or virtual power. The former was applied, for example, by Refs. [21,22] to the case of second- and higher-order hyperelastic continua without microstructure, and more recently in many other works involving generalized continua such as rate-independent strain-gradient plasticity (e.g., [54,55]). More generally, the principle of virtual power has been applied in this vein in many works in mechanics and thermomechanics (e.g., [12,25,56–62]). Such principles are among the most recent examples in the history of mechanics of the quest to "rationalize" it (e.g., [63]), i.e., to cast mechanics (and thermodynamics) in "axiomatic", universally valid, purely mathematical form independent of (any particular) physics.

As attested to, for example, by the current work, rather than postulating such a variational or variational-like relation or "principle" from the start, the second approach *derives* such relations for particular (classes of) models based on physics, thermodynamics, and material theory (e.g., [3,19,20,32,39,41,42,64]). This view on variational "principles" was expressed for example by Truesdell and Toupin [65, §231], who noted that these represent derived entities. If possible, mathematical reformulation of any physical model in variational form obviously provides a number of advantages for the formulation and solution of IBVPs. Such advantages have long been recognized and exploited in material science, chemical thermodynamics, and condensed matter physics (e.g., [17,45–47,51,52]).

Following many previous works [3, Chapters 13–14], a distinction is made in the current work between thermodynamic equilibrium, i.e., states of zero velocity, uniform temperature, and no dissipation, and the more general (non-equilibrium) steady states, which are dissipative due to, e.g., gradients in temperature and velocity. Both equilibrium states and steady states are generally dependent on the environment in which the system finds itself. This issue, the consequences of second-order, and the formulation of configurational field and balance relations based on the Eshelby stress, for the case of extended or generalized crystal plasticity, all represent work in progress to be reported on in the future. This also holds for much more sophisticated approaches that the current "mean-field" one for extended or generalized continua such as those based on distribution functions (e.g., [66–68]) or even statistical mechanics itself (e.g., [69–73]). Among other things, the latter promises significant further insight into the structure of such models and the interpretation of their fields.

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