Continua described by a microstructural field*

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Abstract

Using a balance law for microforces and an appropriate statement of the second law of thermodynamics, a framework is provided for continuum theories that involve a microstructural variable. Examples of specific physical theories that fall within that framework—spanning internal state-variable theories for plasticity and polymeric solutions, order-parameter based theories for phase transitions, and various theories for liquid crystals—are given.

1 Introduction

In this note we give a unified presentation of a class of continuum theories whose central feature is a field introduced to model internal structure. To focus attention on the treatment of such *microstructural fields*, we restrict discussion to a purely mechanical theory and ignore deformation.[1]

In Section 2 we discuss necessary preliminaries concerned with microstructural fields. We then, in Section 3, introduce the basic variables and principles of our theory. The former consist of a system of microforces that act in response to microstructural changes, while the latter consist of a balance that constrains the elements of that force system and a statement of the second law that accounts properly for power expenditures associated with microstructual evolution. In Section 4 we introduce a simple class of constitutive assumptions and deduce, based on the second law, thermodynamic restrictions on those assumptions. Finally, in Section 5, we provide examples of specific physical theories encompassed

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[1] Excepting the addition of suitable requirements concerning invariance with respect to rigid changes in spatial observer, an extension of our approach to include deformational effects requires no significant change in the aspects of the conceptual framework associated with the microstructural field. Thermal and compositional effects are also readily incorporated.

by our framework. These comprise: internal state-variable theories for *plasticity* and *polymeric solutions*; order-parameter based theories for *phase transitions*; and various theories for *liquid crystals.*

2 Microstructural fields

We consider a body with internal structure characterized by a list φ in $\mathbb{R}^M$ of microstructural variables subject to a constraint requiring that φ lie on a smooth surface $\mathcal{S}$ contained in $\mathbb{R}^M$. We write $\mathcal{T}(\varphi)$ for the tangent space to $\mathcal{S}$ at φ of $\mathcal{S}$, $\boldsymbol{P}(\varphi)$ for the projection of $\mathbb{R}^M$ onto $\mathcal{T}(\varphi)$, and $\boldsymbol{N}(\varphi)$ for the projection of $\mathbb{R}^M$ onto $(\mathcal{T}(\varphi))^{\perp}$; $\boldsymbol{P}(\varphi)$ and $\boldsymbol{N}(\varphi)$, respectively, map each list in $\mathbb{R}^M$ into its components tangential and normal to $\mathcal{S}$ at φ.

During an evolution of the body, which we identify with a fixed region $\mathcal{B}$ in $\mathbb{R}^3$, the list of microstructural variables will be a field defined on that region for all time. This microstructural field has values in $\mathcal{S}$, but for the purposes of analysis it is more convenient to consider it as having values in $\mathbb{R}^M$, with gradient

$$\boldsymbol{G} := \nabla\varphi. \tag{2.1}$$

Then $\boldsymbol{G}(\boldsymbol{x},t)$ belongs to $\mathrm{Lin}(\mathbb{R}^3,\mathbb{R}^M)$ at each $(\boldsymbol{x},t)$, but $\boldsymbol{G}$ is tangential in the sense that[2]

$$\boldsymbol{N}(\varphi)\boldsymbol{G} = \boldsymbol{0}. \tag{2.2}$$

Similarly,

$$\boldsymbol{h} := \dot{\varphi} \tag{2.3}$$

is tangential, since

$$\boldsymbol{N}(\varphi)\boldsymbol{h} = \boldsymbol{0} \tag{2.4}$$

(i.e., $\boldsymbol{h}$ is an element of $\mathcal{T}(\varphi)$).

It is convenient to work also with local fields. Precisely, a *local microstructural field* is a smooth field $\varphi : \mathcal{P}\times\mathcal{I} \to \mathcal{S}$ with $\mathcal{P}$ an open subset of $\mathcal{B}$ and $\mathcal{I}$ an open time interval contained in $\mathbb{R}$. The following lemma will be useful in deducing restrictions on constitutive equations.

[2] Given finite-dimensional inner product spaces $\mathcal{V}$ and $\mathcal{W}$, $\mathrm{Lin}(\mathcal{V},\mathcal{W})$ is the space of linear transformations from $\mathcal{V}$ into $\mathcal{W}$; $\mathrm{Lin}(\mathcal{V},\mathcal{W})$ is equipped with inner product $\boldsymbol{A}\cdot\boldsymbol{B} = \mathrm{tr}(\boldsymbol{A}\boldsymbol{B}^{\scriptscriptstyle T})$, where $\boldsymbol{B}^{\scriptscriptstyle T}$ is the transpose of $\boldsymbol{B}$ and $\mathrm{tr}\boldsymbol{B}$ denotes the trace of $\boldsymbol{B}$.

Variation Lemma. Choose φ_0 in $\mathcal{S}$ arbitrarily, and let $\boldsymbol{P}_0 = \boldsymbol{P}(\varphi_0)$ and $\boldsymbol{N}_0 = \boldsymbol{N}(\varphi_0)$. Then given elements $\boldsymbol{G}_0$ and $\boldsymbol{G}_*$ of $\mathrm{Lin}(\mathbb{R}^3, \mathbb{R}^M)$ and elements $\boldsymbol{h}_0$ and $\boldsymbol{h}_*$ of $\mathbb{R}^M$ consistent with

$$\boldsymbol{N}_0\boldsymbol{G}_0 = \boldsymbol{N}_0\boldsymbol{G}_*, \quad \boldsymbol{N}_0\boldsymbol{h}_0 = \boldsymbol{N}_0\boldsymbol{h}_*, \tag{2.5}$$

there is a local microstructural field φ such that, at some $(\boldsymbol{x}_0, t_0)$ in its domain,

$$\varphi(\boldsymbol{x}_0, t_0) = \varphi_0, \quad \boldsymbol{G}(\boldsymbol{x}_0, t_0) = \boldsymbol{G}_0, \quad \boldsymbol{h}(\boldsymbol{x}_0, t_0) = \boldsymbol{h}_0, \tag{2.6}$$

and

$$\boldsymbol{P}_0\dot{\boldsymbol{G}}(\boldsymbol{x}_0, t_0) = \boldsymbol{G}_*, \quad \boldsymbol{P}_0\dot{\boldsymbol{h}}(\boldsymbol{x}_0, t_0) = \boldsymbol{h}_*. \tag{2.7}$$

Proof. Since $\mathcal{S}$ is a smooth surface in $\mathbb{R}^M$, we can find a smooth function $\boldsymbol{f}$ from an open set $\mathcal{A}$ in $\mathbb{R}^{M-1}$ onto a neighborhood $\mathcal{N}$ of φ_0 such that, at each $\boldsymbol{w}$ in $\mathcal{A}$, the derivative $D\boldsymbol{f}(\boldsymbol{w})$, which is an element of $\mathrm{Lin}(\mathbb{R}^{M-1}, \mathbb{R}^M)$, maps $\mathbb{R}^{M-1}$ invertibly onto $\mathcal{T}(\boldsymbol{f}(\boldsymbol{w}))$. Choose $(\boldsymbol{x}_0, t_0)$ and let $\boldsymbol{w} : \mathcal{P} \times \mathcal{I} \to \mathcal{A}$, where $\mathcal{P}$ is an open subset of $\mathcal{B}$ containing $\boldsymbol{x}_0$ and $\mathcal{I}$ is an open interval containing t_0, and $\boldsymbol{w}_0 := \boldsymbol{w}(\boldsymbol{x}_0, t_0) = \boldsymbol{f}^{-1}(\varphi_0)$. Then, upon writing $\varphi(\boldsymbol{x}, t) = \boldsymbol{f}(\boldsymbol{w}(\boldsymbol{x}, t))$,

$$\left.\begin{aligned}
\boldsymbol{G} &= D\boldsymbol{f}(\boldsymbol{w})\nabla\boldsymbol{w}, \\
\boldsymbol{h} &= D\boldsymbol{f}(\boldsymbol{w})\dot{\boldsymbol{w}}, \\
\dot{\boldsymbol{G}} &= D\boldsymbol{f}(\boldsymbol{w})\nabla\dot{\boldsymbol{w}} \quad \text{plus a function of } (\boldsymbol{w}, \dot{\boldsymbol{w}}, \nabla\boldsymbol{w}), \\
\dot{\boldsymbol{h}} &= D\boldsymbol{f}(\boldsymbol{w})\ddot{\boldsymbol{w}} \quad \text{plus a function of } (\boldsymbol{w}, \dot{\boldsymbol{w}}).
\end{aligned}\right\} \tag{2.8}$$

Consider the requirements (2.6) and (2.7). Since $D\boldsymbol{f}(\boldsymbol{w})$ maps $\mathbb{R}^{M-1}$ invertibly onto $\mathcal{T}(\boldsymbol{f}(\boldsymbol{w}))$, we can find $\dot{\boldsymbol{w}}(\boldsymbol{x}_0, t_0)$ and $\nabla\boldsymbol{w}(\boldsymbol{x}_0, t_0)$ such that $\boldsymbol{G}(\boldsymbol{x}_0, t_0)$ and $\boldsymbol{h}(\boldsymbol{x}_0, t_0)$ have the requisite values, and granted this, we can find $\ddot{\boldsymbol{w}}(\boldsymbol{x}_0, t_0)$ and $\nabla\dot{\boldsymbol{w}}(\boldsymbol{x}_0, t_0)$ such that $\boldsymbol{P}_0\dot{\boldsymbol{G}}(\boldsymbol{x}_0, t_0)$ and $\boldsymbol{P}_0\dot{\boldsymbol{h}}(\boldsymbol{x}_0, t_0)$ do also. Since we can always construct a smooth field $\boldsymbol{w} : \mathcal{P} \times \mathcal{I} \to \mathcal{A}$ for which $\boldsymbol{w}$, $\dot{\boldsymbol{w}}$, $\nabla\boldsymbol{w}$, $\ddot{\boldsymbol{w}}$, and $\nabla\dot{\boldsymbol{w}}$ have arbitrarily prescribed values at $(\boldsymbol{x}_0, t_0)$, the lemma follows.

3 Microforce balance. Dissipation inequality

3.1 Microforce balance

We associate with each evolution of $\mathcal{B}$ a microstructural force system that acts in response to changes in φ. This force system consists, at each $(\boldsymbol{x}, t)$, of a *stress*

$\boldsymbol{\Sigma}(\boldsymbol{x},t)$ in $\mathrm{Lin}(\mathbb{R}^3,\mathbb{R}^M)$, an *internal force* $\boldsymbol{\pi}(\boldsymbol{x},t)$ in $\mathbb{R}^M$, and an *external force* $\boldsymbol{\gamma}(\boldsymbol{x},t)$ in $\mathbb{R}^M$, with $\boldsymbol{\Sigma}$, $\boldsymbol{\pi}$, and $\boldsymbol{\gamma}$ tangential, viz.

$$\boldsymbol{N}(\boldsymbol{\varphi})\boldsymbol{\Sigma} = \mathbf{0}, \quad \boldsymbol{N}(\boldsymbol{\varphi})\boldsymbol{\pi} = \mathbf{0}, \quad \boldsymbol{N}(\boldsymbol{\varphi})\boldsymbol{\gamma} = \mathbf{0}. \tag{3.1}$$

A major premise of our theory is that this force system is consistent with the *microforce balance*

$$\int\limits_{\partial\mathcal{P}} \boldsymbol{\Sigma}\boldsymbol{\nu}\, da + \int\limits_{\mathcal{P}} (\boldsymbol{\pi} + \boldsymbol{\gamma})\, dv = \mathbf{0} \tag{3.2}$$

for all subregions $\mathcal{P}$ of $\mathcal{B}$ and all time, where $\boldsymbol{\nu}$ is the unit outward normal to $\partial\mathcal{P}$.[3] The balance (3.2) has the local form

$$\mathrm{div}\,\boldsymbol{\Sigma} + \boldsymbol{\pi} + \boldsymbol{\gamma} = \mathbf{0}, \tag{3.3}$$

where, given any constant list $\boldsymbol{a}$ in $\mathbb{R}^M$, $\mathrm{div}\,\boldsymbol{\Sigma}$ is defined by the relation

$$\boldsymbol{a}\cdot\mathrm{div}\,\boldsymbol{\Sigma} = \mathrm{div}(\boldsymbol{\Sigma}^{\mathsf{T}}\boldsymbol{a}). \tag{3.4}$$

3.2 Dissipation inequality

Since thermal and deformational effects are suppressed, the second law is the assertion that the free energy of any subregion $\mathcal{P}$ may not increase at a rate that exceeds the working of all forces *external* to $\mathcal{P}$. Granted our premise that the microstructural forces act in response to changes to the microstructural variable, that working is given by

$$\int\limits_{\partial\mathcal{P}} \boldsymbol{\Sigma}\boldsymbol{\nu}\cdot\dot{\boldsymbol{\varphi}}\, da + \int\limits_{\mathcal{P}} \boldsymbol{\gamma}\cdot\dot{\boldsymbol{\varphi}}\, dv. \tag{3.5}$$

Thus, letting ψ denote the *free energy* (per unit volume), we write the second law in the form of a dissipation inequality

$$\overline{\int\limits_{\mathcal{P}} \psi\, dv}^{\,\boldsymbol{\cdot}} \le \int\limits_{\partial\mathcal{P}} \boldsymbol{\Sigma}\boldsymbol{\nu}\cdot\dot{\boldsymbol{\varphi}}\, da + \int\limits_{\mathcal{P}} \boldsymbol{\gamma}\cdot\dot{\boldsymbol{\varphi}}\, dv, \tag{3.6}$$

required to hold on all subregions $\mathcal{P}$ of $\mathcal{B}$ and all time. We emphasize that the working (3.5), and hence the dissipation inequality (3.6), does not include a term involving $\boldsymbol{\pi}$, which acts internally to $\mathcal{P}$.

[3] For convenience, we do not include inertial terms in (3.2), although in some applications, for example to ferroelectrics (cf. GORDON & GENOSSAR [1]) and liquid crystals (cf. Ericksen [2]), it might be appropriate to do so; their inclusion involves no added difficulties.

Using (3.3) to eliminate the external force γ from the local version

$$\dot{\psi} \leq \operatorname{div}(\boldsymbol{\Sigma}^T\dot{\boldsymbol{\varphi}}) + \boldsymbol{\pi}\cdot\dot{\boldsymbol{\varphi}} \tag{3.7}$$

of (3.6), we arrive at the local dissipation inequality

$$\dot{\psi} - \boldsymbol{\Sigma}\cdot\dot{\boldsymbol{G}} + \boldsymbol{\pi}\cdot\boldsymbol{h} \leq 0. \tag{3.8}$$

The field

$$\delta := -\dot{\psi} + \boldsymbol{\Sigma}\cdot\dot{\boldsymbol{G}} - \boldsymbol{\pi}\cdot\boldsymbol{h} \geq 0 \tag{3.9}$$

represents *dissipation.* A straightforward but important consequence of the dissipation inequality (3.6), the microforce balance (3.3), and (3.9) is the Lyapunov relation

$$\overline{\int_{\mathcal{B}} \psi\, dv}^{\;\cdot} = -\int_{\mathcal{B}} \delta\, dv \leq 0, \tag{3.10}$$

which holds for the body $\mathcal{B}$ whenever $\boldsymbol{\Sigma\nu}\cdot\dot{\boldsymbol{\varphi}}$ vanishes on $\partial\mathcal{B}$ and γ vanishes on $\mathcal{B}$.

4 Constitutive theory

4.1 Constitutive equations

For constitutive equations we assume that

$$\psi = \hat{\psi}(\boldsymbol{\varphi}, \boldsymbol{G}, \boldsymbol{h}), \quad \boldsymbol{\Sigma} = \hat{\boldsymbol{\Sigma}}(\boldsymbol{\varphi}, \boldsymbol{G}, \boldsymbol{h}), \quad \boldsymbol{\pi} = \hat{\boldsymbol{\pi}}(\boldsymbol{\varphi}, \boldsymbol{G}, \boldsymbol{h}). \tag{4.1}$$

We do not write a constitutive equation for the external force γ, but instead allow it to be assigned in any manner compatible with the microforce balance.

The domain of each of the response functions $\hat{\psi}$, $\hat{\boldsymbol{\Sigma}}$, and $\hat{\boldsymbol{\pi}}$ is the set of all $(\boldsymbol{\varphi}, \boldsymbol{G}, \boldsymbol{h})$ such that $\boldsymbol{\varphi}$ is an element of $\mathcal{S}$, $\boldsymbol{G}$ is an element of $\mathrm{Lin}(\mathbb{R}^3, \mathbb{R}^M)$, and $\boldsymbol{h}$ is an element of $\mathbb{R}^M$, with $\boldsymbol{G}$ and $\boldsymbol{h}$ tangential. Because of the dependence of this latter requirement on $\boldsymbol{\varphi}$ (cf. (2.2) and (2.4)), the partial derivatives of $\hat{\psi}(\boldsymbol{\varphi}, \boldsymbol{G}, \boldsymbol{h})$ are complicated to define. To avoid such difficulties we extend the response functions as follows: given a response function $\hat{f}$, we introduce

$$\tilde{f}(\boldsymbol{\varphi}, \boldsymbol{G}, \boldsymbol{h}) = \hat{f}(\boldsymbol{\varphi}, \boldsymbol{P}(\boldsymbol{\varphi})\boldsymbol{G}, \boldsymbol{P}(\boldsymbol{\varphi})\boldsymbol{h}); \tag{4.2}$$

then $\tilde{f}(\varphi, \boldsymbol{G}, \boldsymbol{h})$ is defined for all φ in $\mathcal{S}$, $\boldsymbol{G}$ in $\mathrm{Lin}(\mathbb{R}^3, \mathbb{R}^M)$, and $\boldsymbol{h}$ in $\mathbb{R}^M$, irrespective of whether $\boldsymbol{G}$ and $\boldsymbol{h}$ are tangential. Because of (4.2),

$$\left.\begin{aligned} \boldsymbol{N}(\varphi)\partial_\varphi\tilde{\psi}(\varphi, \boldsymbol{G}, \boldsymbol{h}) &= \boldsymbol{0}, \\ \boldsymbol{N}(\varphi)\partial_{\boldsymbol{G}}\tilde{\psi}(\varphi, \boldsymbol{G}, \boldsymbol{h}) &= \boldsymbol{0}, \\ \boldsymbol{N}(\varphi)\partial_{\boldsymbol{h}}\tilde{\psi}(\varphi, \boldsymbol{G}, \boldsymbol{h}) &= \boldsymbol{0}, \end{aligned}\right\} \tag{4.3}$$

and similar restrictions apply to the other response functions.[4]

4.2 Thermodynamic restrictions

Following Coleman & Noll [3], we assume that given any local microstructural field, the corresponding constitutive process defined by (4.1) is consistent with the dissipation inequality (3.8). Substituting (4.1) into (3.8) yields

$$\boldsymbol{a}(\varphi, \boldsymbol{G}, \boldsymbol{h})\cdot\boldsymbol{h} + \boldsymbol{A}(\varphi, \boldsymbol{G}, \boldsymbol{h})\cdot\dot{\boldsymbol{G}} + \boldsymbol{b}(\varphi, \boldsymbol{G}, \boldsymbol{h})\cdot\dot{\boldsymbol{h}} \leq 0 \tag{4.4}$$

with

$$\left.\begin{aligned} \boldsymbol{a}(\varphi, \boldsymbol{G}, \boldsymbol{h}) &= \partial_\varphi\tilde{\psi}(\varphi, \boldsymbol{G}, \boldsymbol{h}) - \tilde{\boldsymbol{\pi}}(\varphi, \boldsymbol{G}, \boldsymbol{h}), \\ \boldsymbol{A}(\varphi, \boldsymbol{G}, \boldsymbol{h}) &= \partial_{\boldsymbol{G}}\tilde{\psi}(\varphi, \boldsymbol{G}, \boldsymbol{h}) - \tilde{\boldsymbol{\Sigma}}(\varphi, \boldsymbol{G}, \boldsymbol{h}), \\ \boldsymbol{b}(\varphi, \boldsymbol{G}, \boldsymbol{h}) &= \partial_{\boldsymbol{h}}\tilde{\psi}(\varphi, \boldsymbol{G}, \boldsymbol{h}), \end{aligned}\right\} \tag{4.5}$$

and where, by (3.1) and (4.3),

$$\left.\begin{aligned} \boldsymbol{N}(\varphi)\boldsymbol{a}(\varphi, \boldsymbol{G}, \boldsymbol{h}) &= \boldsymbol{0}, \\ \boldsymbol{N}(\varphi)\boldsymbol{A}(\varphi, \boldsymbol{G}, \boldsymbol{h}) &= \boldsymbol{0}, \\ \boldsymbol{N}(\varphi)\boldsymbol{b}(\varphi, \boldsymbol{G}, \boldsymbol{h}) &= \boldsymbol{0}. \end{aligned}\right\} \tag{4.6}$$

The variation lemma, (4.5), and (4.6) yield the conclusions $\boldsymbol{A}(\varphi, \boldsymbol{G}, \boldsymbol{h}) = \boldsymbol{0}$ and $\boldsymbol{b}(\varphi, \boldsymbol{G}, \boldsymbol{h}) = \boldsymbol{0}$; hence

$$\left.\begin{aligned} \partial_{\boldsymbol{h}}\tilde{\psi}(\varphi, \boldsymbol{G}, \boldsymbol{h}) &= \boldsymbol{0}, \\ \tilde{\boldsymbol{\Sigma}}(\varphi, \boldsymbol{G}, \boldsymbol{h}) &= \partial_{\boldsymbol{G}}\tilde{\psi}(\varphi, \boldsymbol{G}, \boldsymbol{h}), \\ \big(\partial_\varphi\tilde{\psi}(\varphi, \boldsymbol{G}, \boldsymbol{h}) - \tilde{\boldsymbol{\pi}}(\varphi, \boldsymbol{G}, \boldsymbol{h})\big)&\cdot\boldsymbol{h} \leq 0. \end{aligned}\right\} \tag{4.7}$$

We therefore have the following result.

[4] Here, for example, $\partial_{\boldsymbol{h}}\tilde{\psi}(\varphi, \boldsymbol{G}, \boldsymbol{h})$ denotes the value at $(\varphi, \boldsymbol{G}, \boldsymbol{h})$ of the partial derivative of $\tilde{\psi}$ with respect to $\boldsymbol{h}$.

Thermodynamic restrictions. The response functions $\tilde{\psi}$ and $\tilde{\boldsymbol{\Sigma}}$ are independent of $\boldsymbol{h}$ and satisfy

$$\tilde{\boldsymbol{\Sigma}}(\varphi, \boldsymbol{G}) = \partial_{\boldsymbol{G}}\tilde{\psi}(\varphi, \boldsymbol{G}), \tag{4.8}$$

while $\tilde{\pi}$ has the form[5]

$$\tilde{\pi}(\varphi, \boldsymbol{G}, \boldsymbol{h}) = -\partial_{\varphi}\tilde{\psi}(\varphi, \boldsymbol{G}) - \boldsymbol{B}(\varphi, \boldsymbol{G}, \boldsymbol{h})\boldsymbol{h}, \tag{4.9}$$

with $\boldsymbol{B}(\varphi, \boldsymbol{G}, \boldsymbol{h})$, the *kinetic modulus*, a linear transformation from $\mathcal{T}(\varphi)$ into itself that, by virtue of $(4.7)_{1,2}$, (4.9), and (3.9), must be consistent with

$$\boldsymbol{h}\cdot\boldsymbol{B}(\varphi, \boldsymbol{G}, \boldsymbol{h})\boldsymbol{h} = \delta \geq 0, \tag{4.10}$$

for all $\boldsymbol{h}$ in $\mathcal{T}(\varphi)$.

Combining the balance law (3.3) and the constitutive equations (4.8) and (4.9) yields

$$\boldsymbol{B}(\varphi, \boldsymbol{G}, \dot{\varphi})\dot{\varphi} = \operatorname{div}\left(\partial_{\boldsymbol{G}}\tilde{\psi}(\varphi, \boldsymbol{G})\right) - \partial_{\varphi}\tilde{\psi}(\varphi, \boldsymbol{G}) + \gamma, \tag{4.11}$$

the governing equation of our theory for a continuum with internal structure described by the microstructural field φ.

5 Examples

We now list specific physical theories that are special cases of the general theory discussed above. We assume throughout that the external force γ vanishes.

5.1 Internal state-variables

If we assume that $\tilde{\psi}$ is independent of $\boldsymbol{G} = \nabla\varphi$ and take $\boldsymbol{B}$ to be the identity on $\mathcal{T}(\varphi)$, then (4.11) reduces to

$$\dot{\varphi} = -\partial_{\varphi}\tilde{\psi}(\varphi), \tag{5.1}$$

which is a standard rate law for an *internal state-variable* φ (cf., e.g., COLEMAN & GURTIN [5]). Within internal variable theories for plasticity (cf., e.g., KRATOCHVIL & DILLON [6], LUBLINER [7], RICE [8]) and for polymeric solutions (cf., e.g., HAND [9], DASHNER & VANARSDALE [10], MAUGIN & DROUOT [11]), φ describes material microstructure and $-\partial_{\varphi}\tilde{\psi}(\varphi)$ is a thermodynamic

5 Granted smoothness of the response functions, (4.9) provides the most general representation for $\tilde{\pi}$ consistent with $(4.7)_3$ (cf. the lemma of GURTIN & VOORHEES [4]).

force that is power-conjugate to microstructural rearrangement, an interpretation that renders the derivation of (5.1) based on a force balance more appealing than the standard approach in which it is viewed as a constitutive rate equation.[6] From our perspective, equation (5.1) simply enforces the requirement that the equilibrium and dissipative contributions to the internal microforce must be of equal magnitude but opposite direction on $\mathcal{T}(\varphi)$.

5.2 Order parameters

If we let $\mathcal{S} \subset \mathbb{R}$, so that the microstructural variable and the kinetic coefficient are both scalars, which we denote respectively by φ and β, and assume that $\tilde{\psi}$ has the form

$$\tilde{\psi}(\varphi, \nabla\varphi) = f(\varphi) + \tfrac{1}{2}\lambda|\nabla\varphi|^2, \qquad \lambda > 0, \tag{5.2}$$

then (4.11) reduces to the Allen-Cahn-Ginzburg-Landau equation

$$\beta\dot{\varphi} = \lambda\Delta\varphi - \partial_\varphi f(\varphi). \tag{5.3}$$

This equation—with φ interpreted as an *order parameter* and f a double-well potential—is often used to describe the evolution of boundaries between phases (cf., e.g., CHAN [13], ALLEN & CAHN [14]). The foregoing derivation based on a microforce balance, a dissipation inequality, and suitable constitutive equations is due to FRIED & GURTIN [15].[7]

5.3 Directors

If we take $\mathcal{S}$ to be the unit sphere $\mathbb{S}^2$ in $\mathbb{R}^3$, write $\boldsymbol{n}$ for the microstructural variable, take $\boldsymbol{B}$ to be proportional, by a positive scalar β, to the identity on $\mathcal{T}(\boldsymbol{n})$, and let

$$\hat{\psi}(\boldsymbol{n}, \nabla\boldsymbol{n}) = \tfrac{1}{2}\lambda|\nabla\boldsymbol{n}|^2, \qquad \lambda > 0; \tag{5.4}$$

then, bearing in mind the definition (4.2) of an extended response function, (4.11) yields a simple version of the evolution equation governing the *director*

[6] Evolution equations of the form (5.1) have also been proposed within theories of chemical reactions (cf. DE DONDER & VAN RYSSELBERGHE [12]), in which case φ and $-\partial_\varphi\tilde{\psi}(\varphi)$, respectively, represent lists with q-th components the *degree of advancement* and *affinity* of the q-th reaction.

[7] See also FRIED & GURTIN [16], who generalize (5.2) and (5.3) to include deformation with $M > 1$ and $\mathcal{S}$ an affine subset of $\mathbb{R}^M$, and GURTIN, POLIGNONE & VIÑALS [17], who generalize (5.2) and (5.3) to account for flow.

$\boldsymbol{n}$ in the Ericksen-Leslie theory of uniaxial nematic liquid crystals:

$$\beta\dot{\boldsymbol{n}} = \lambda(\Delta\boldsymbol{n} + |\nabla\boldsymbol{n}|^2\boldsymbol{n}). \tag{5.5}$$

More generally, if we identify $\mathcal{S}$ with $\mathbb{S}^2 \times [-\frac{1}{2}, 1]$, write $(\boldsymbol{n}, s)$ for the microstructural variable, denote $\nabla\boldsymbol{n}$ and ∇s by $\boldsymbol{G}$ and $\boldsymbol{g}$, and take $\boldsymbol{B}$ to be a proportional, once again by a positive scalar β, to the identity on $\mathcal{T}(\boldsymbol{n}, s)$, then the evolution equations fall within those given by ERICKSEN [2] in his recent theory for uniaxial liquid crystals with variable degree of orientation:

$$\left.\begin{aligned} \beta\dot{\boldsymbol{n}} &= \operatorname{div}\big(\partial_{\boldsymbol{G}}\tilde{\psi}(\boldsymbol{n}, \boldsymbol{G}, s, \boldsymbol{g})\big) - \partial_{\boldsymbol{n}}\tilde{\psi}(\boldsymbol{n}, \boldsymbol{G}, s, \boldsymbol{g}), \\ \beta\dot{s} &= \operatorname{div}\big(\partial_{\boldsymbol{g}}\tilde{\psi}(\boldsymbol{n}, \boldsymbol{G}, s, \boldsymbol{g})\big) - \partial_{s}\tilde{\psi}(\boldsymbol{n}, \boldsymbol{G}, s, \boldsymbol{g}), \end{aligned}\right\} \tag{5.6}$$

with $\boldsymbol{n}$ the *director* and s the *degree of orientation.*

Under a simple generalization

$$\left.\begin{aligned} \hat{\psi}(\boldsymbol{n}, \nabla\boldsymbol{n}, s, \nabla s) = f(s) + \tfrac{1}{2}\lambda s^2|\nabla\boldsymbol{n}|^2 + \tfrac{1}{2}\mu|\nabla s|^2, \\ \lambda > 0, \quad \mu > 0, \end{aligned}\right\} \tag{5.7}$$

of (5.4) proposed by VIRGA [18], where f is a double-well potential with local minima at $s = 0$ and $s = s_*$, with $0 < s_* < 1$,[8] the system (5.6) reduces to

$$\left.\begin{aligned} \beta\dot{\boldsymbol{n}} &= \lambda(\operatorname{div}(s^2\nabla\boldsymbol{n}) + s^2|\nabla\boldsymbol{n}|^2\boldsymbol{n}), \\ \beta\dot{s} &= \mu\Delta s - \lambda s|\nabla\boldsymbol{n}|^2 - \partial_s f(s), \end{aligned}\right\} \tag{5.8}$$

yielding a modification of (5.5) that incorporates a coupling to Allen-Cahn-Ginzburg-Landau dynamics (cf. (5.3)) and, hence, an ability to model isotropic-nematic transitions.

5.4 Alignment tensors

If we take $\mathcal{S}$ to be the set containing all symmetric and traceless elements of $\mathrm{Lin}(\mathbb{R}^3, \mathbb{R}^3)$, denote the microstructural variable by $\boldsymbol{Q}$, let $\boldsymbol{B}$ be proportional to the identity on $\mathcal{T}(\boldsymbol{Q})$, and suppose that

$$\hat{\psi}(\boldsymbol{Q}, \nabla\boldsymbol{Q}) = f(\boldsymbol{Q}) + \tfrac{1}{2}\lambda|\nabla\boldsymbol{Q}|^2, \qquad \lambda > 0, \tag{5.9}$$

with f, as given for example by DE GENNES [19], then (4.11) yields a tensorial analogue of (5.3) that encompasses biaxiality and is able to describe a broad range of phase transitions.

[8] The values $s = 0$ and $s = 1$ for the degree of orientation correspond, respectively, to random and perfect alignment.

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