Chapter 16
Use and Abuse of the Method of Virtual Power in Generalized Continuum Mechanics and Thermodynamics

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Abstract The method of virtual power, put forward by Paul Germain and celebrated by Gérard A. Maugin, is *used* (and *abused*) in the present work in combination with continuum thermodynamics concepts in order to develop generalized continuum, phase field, higher order temperature and diffusion theories. The systematic and effective character of the method is illustrated in the case of gradient and micromorphic plasticity models. It is then tentatively applied to the introduction of temperature and concentration gradient effects in diffusion theories leading to generalized heat and mass diffusion equations.

16.1 Introduction

There are essentially two equivalent ways to mathematically represent forces acting on continuum mechanical media: the introduction of forces and couples in the balance of moment and moment of momentum equations, on the one hand, and the method of virtual power, on the other hand, which is a variational statement of the dynamics of bodies (Germain, 1973a). The axiomatic and systematic character of the latter has been put forward by P. Germain and illustrated in the case of first and second gradient continuum theories. It has the merit of clearly separating universal balance laws from peculiar constitutive laws in contrast to Lagrangian/Hamiltonian mechanics which was used by Mindlin to first propose a consistent strain gradient elasticity theory with suitable boundary conditions (Mindlin, 1965). The derivation of complex boundary conditions as they arise in strain gradient and also plate theories probably is the most striking example where the method of virtual power is undoubtedly more effective than the usual procedure. This is due to the fact that the complex form of contact forces, in contrast to internal forces, can hardly be anticipated in that case,

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as discussed in dell'Isola and Seppecher (1995); dell'Isola et al (2012). Following Germain, Maugin has promoted the method of virtual power and extended it to non–mechanical fields in order to construct complex and coupled continuum theories (Maugin, 1980). The latter contribution deals with the coupling of mechanics with electromagnetism. Maugin also introduced the consideration of singular surfaces and interfaces for mechanical and thermodynamic field variables (Daher and Maugin, 1986). Maugin's passion for the method of virtual power in continuum physics led him recently to write a review paper on the merits of the approach and the many fields of application, namely mechanics of one, two and three–dimensional continuum mechanics, including beam, plate and shell theories, and the coupling with electromagnetic fields (Maugin, 2013).

The mechanics of generalized continua is undoubtedly the privileged domain of application of the principle of virtual power because it enables the systematic introduction of enriched kinematics of the material point with the conjugate forces. This is illustrated by the application of this method to the theory of micromorphic media by Germain (1973b). As claimed by Germain, the derived balance laws and boundary conditions were not new but the level of generality was increased by the systematic nature of the method and the definition by Germain of general micromorphic continua with additional degrees of freedom represented by tensors of increasing order. The method is illustrated in several recent books edited by G.A. Maugin and collecting various generalized continuum theories (Maugin and Metrikine, 2010; Altenbach et al, 2011).

The combination of the method of virtual power and the concepts of continuum thermodynamics, again following Germain's incentive (Germain et al, 1983), leads to a complete framework for the development of continuum theories including consistent constitutive equations. Within this framework, Maugin himself significantly developed the thermomechanics of continua (Maugin, 1992, 1999). He recently also applied the method to coupled diffusion theory (Maugin, 2006).

The objective of the present work is first to extend generalized continuum approaches like strain gradient and micromorphic models to plasticity and damage by means of the method of virtual power and continuum thermodynamics. This shows the systematic *use* and the merits of the method. The second part deals with the coupling of the mechanics with thermodynamic fields like temperature, phase field and concentration. The attention is drawn on the introduction of the gradient of these variables into thermodynamic potentials. For that purpose, the method of virtual power is used again in non-conventional situations, which may represent an *abuse* of the method in the sense that its application may be regarded as formal. It however delivers new types of balance and evolution equations that can be compared to more standard formulations. In particular, the two last sections deal with the application of the method of virtual power to the construction of phase field and higher order diffusion models. These formulations differ from the classical ones based on variational derivatives that do not take enough care of boundary conditions. The seminal contribution by Gurtin (1996) proposes a construction of the phase field continuum theory using additional balance laws for so–called microstress and

microforce tensors. In the present work, the method of virtual power is used instead and applied to various situations.

An intrinsic notation system is used in this chapter whereby tensors of order 1, 2 and 4 are respectively denoted by $\underline{a}$, $\underset{\sim}{A}$ and $\underset{\approx}{A}$. Simple and double contractions read:

$$\underline{f} \cdot \underline{v} = f_i v_i, \quad \underset{\sim}{A} : \underset{\sim}{B} = A_{ij} B_{ij} \tag{16.1}$$

The gradient and divergence operators are written as

$$\nabla \underline{u} = u_{i,j}\, \underline{e}_i \otimes \underline{e}_j, \quad \underset{\sim}{\sigma} \cdot \nabla = \sigma_{ij,j}\underline{e}_i \tag{16.2}$$

in a Cartesian orthonormal basis $(\underline{e}_1, \underline{e}_2, \underline{e}_3)$.

All theories are presented within the small deformation framework for the sake of brevity. The readers are referred to Forest (2016) for the finite deformation formulations of some of them.

16.2 Micromorphic and Gradient Plasticity

The method of virtual power certainly is an powerful tool to construct generalized continuum mechanics theories ranging from strain gradient to micromorphic continua. Higher order or generalized stresses are introduced via the power density of internal forces and lead to additional boundary conditions for the partial differential equations to be solved. More recently, reduced models have been developed that concentrate the gradient effects on plastic or damage variables instead of the full kinematics (Aifantis, 1984; Frémond and Nedjar, 1996; Gurtin, 2003; Forest, 2009). A generic example is provided in this section dealing with micromorphic and strain gradient plasticity. It can be readily extended to microdamage and gradient damage models (Aslan et al, 2011). The present theory is limited to the quasi-static problem but dynamic contributions of the micromorphic variables can be included as proposed in Saanouni and Hamed (2013).

16.2.1 The Micromorphic Approach to Gradient Plasticity

Within the framework of thermomechanics with additional degrees of freedom (Maugin, 1990), the displacement degrees of freedom, $\underline{u}$, of the material point are complemented by a micromorphic degree of freedom, called here plastic microstrain, p_χ. Within a first gradient theory, the model variables are the strain tensor, $\underset{\sim}{\varepsilon}$, temperature T, internal variables α, the plastic microstrain and its gradient, $p_\chi, \nabla p_\chi$.

The virtual power of internal forces in a subdomain $\mathscr{D}$ of the body $\mathscr{B}$ is a linear form with respect to the degrees of freedom ant their gradients:

$$\mathscr{P}^{(i)}(\underline{v}^{\star}, \dot{p}_{\chi}^{\star}) = - \int_{\mathscr{D}} p^{(i)}(\underline{v}^{\star}, \dot{p}_{\chi}^{\star}) \, dV$$

$$p^{(i)}(\underline{v}^{\star}, \dot{p}_{\chi}^{\star}) = \underset{\sim}{\sigma} : \nabla \underline{v}^{\star} + a \dot{\phi}_{\chi}^{\star} + \underline{b} \cdot \nabla \dot{p}_{\chi}^{\star} \tag{16.3}$$

where $\underline{v}^{\star}, \dot{p}_{\chi}^{\star}$ are virtual velocity and plastic microstrain rate variables. The dual quantities are generalized stresses. The Cauchy stress is $\underset{\sim}{\sigma}$ and a and $\underline{b}$ are generalized stresses associated with the micromorphic variable and its first gradient. Similarly, the power of contact forces must be extended as follows:

$$\mathscr{P}^{(c)}(\underline{v}^{\star}, \dot{p}_{\chi}^{\star}) = \int_{\mathscr{D}} p^{(c)}(\underline{v}^{\star}, \dot{p}_{\chi}^{\star}) \, dV, \quad p^{(c)}(\underline{v}^{\star}, \dot{p}_{\chi}^{\star}) = \underline{t} \cdot \underline{v}^{\star} + a^{c} \dot{p}_{\chi}^{\star} \tag{16.4}$$

where $\underline{t}$ is the traction vector and a^{c} a generalized traction. For conciseness, we do not extend the power of forces acting at a distance and keep the classical form:

$$\mathscr{P}^{(e)}(\underline{v}^{\star}, \dot{p}_{\chi}^{\star}) = \int_{\mathscr{D}} p^{(e)}(\underline{v}^{\star}, \dot{p}_{\chi}^{\star}) \, dV, \quad p^{(e)}(\underline{v}^{\star}, \dot{p}_{\chi}^{\star}) = \rho \underline{f} \cdot \underline{v}^{\star} \tag{16.5}$$

where $\rho \underline{f}$ accounts for given simple body forces. Following Germain (1973a), given body couples and double forces working with the gradient of the velocity field could also be introduced in the theory. The generalized principle of virtual power with respect to the velocity and micromorphic variable fields, is presented here in the static case only:

$$\mathscr{P}^{(i)}(\underline{v}^{\star}, \dot{p}_{\chi}^{\star}) + \mathscr{P}^{(e)}(\underline{v}^{\star}, \dot{p}_{\chi}^{\star}) + \mathscr{P}^{(c)}(\underline{v}^{\star}, \dot{p}_{\chi}^{\star}) = 0, \quad \forall \mathscr{D} \subset \mathscr{B}, \quad \forall \underline{v}^{\star}, \dot{p}_{\chi}^{\star} \tag{16.6}$$

The method of virtual power according to Maugin (1980) is used then to derive the standard local balance of momentum equation:

$$\operatorname{div} \underset{\sim}{\sigma} + \rho \underline{f} = 0, \quad \forall \underline{x} \in \mathscr{B} \tag{16.7}$$

and the generalized balance of micromorphic momentum equation:

$$\operatorname{div} \underline{b} - a = 0, \quad \forall \underline{x} \in \mathscr{B} \tag{16.8}$$

The method also delivers the associated boundary conditions for the simple and generalized tractions:

$$\underline{t} = \underset{\sim}{\sigma} \cdot \underline{n}, \quad a^{c} = \underline{b} \cdot \underline{n}, \quad \forall \underline{x} \in \partial \mathscr{D} \tag{16.9}$$

The local balance of energy is also enhanced by the generalized micromorphic power already included in the power of internal forces (16.3):

$$\rho \dot{e} = p^{(i)} - \operatorname{div} \underline{q} \tag{16.10}$$

where ϵ is the specific internal energy and $\underset{\sim}{q}$ the heat flux vector. The entropy principle takes the usual local form:

$$-\rho(\dot{\psi} + \eta\dot{T}) + p^{(i)} - \frac{q}{T}.\nabla T \geq 0 \qquad (16.11)$$

where it is assumed that the entropy production vector is still equal to the heat vector divided by temperature, as in classical thermomechanics according to Coleman and Noll (1963). Again, the enhancement of the theory goes through the enriched power density of internal forces (16.3). The entropy principle is exploited according to classical continuum thermodynamics to derive the state laws. At this stage it is necessary to be more specific on the dependence of the state functions $\psi, \eta, \underset{\sim}{\sigma}, a, \underline{b}$ on state variables and to distinguish between dissipative and non–dissipative mechanisms. The introduction of dissipative mechanisms may require an increase in the number of state variables. The presentation is limited here to non–dissipative contributions of generalized stresses (see Forest, 2009; Aslan and Forest, 2011) for more sophisticated cases including dissipative contributions). Dissipative events are assumed here to enter the model only via the classical mechanical part. Total strain is split into elastic and plastic parts:

$$\underset{\sim}{\varepsilon} = \underset{\sim}{\varepsilon}^e + \underset{\sim}{\varepsilon}^p \qquad (16.12)$$

The constitutive functional are assumed to depend on the following set of state variables:

$$(\underset{\sim}{\varepsilon}^e, T, \alpha, p_\chi, \nabla p_\chi)$$

The entropy inequality (16.11) can be expanded as:

$$(\underset{\sim}{\sigma} - \rho\frac{\partial\psi}{\partial\underset{\sim}{\varepsilon}^e}) : \dot{\underset{\sim}{\varepsilon}}^e + \rho(\eta + \frac{\partial\psi}{\partial T})\dot{T} + (a - \rho\frac{\partial\psi}{\partial p_\chi})\dot{p}_\chi + (\underline{b} - \rho\frac{\partial\psi}{\partial\nabla p_\chi}) \cdot \nabla\dot{p}_\chi$$

$$+ \underset{\sim}{\sigma} : \dot{\underset{\sim}{\varepsilon}}^p - \rho\frac{\partial\psi}{\partial\alpha}\dot{\alpha} - \frac{q}{T} \cdot \nabla T \geq 0 \qquad (16.13)$$

Assuming that no dissipation is associated with the four first terms of the previous inequality, the following state laws are found

$$\underset{\sim}{\sigma} = \rho\frac{\partial\psi}{\partial\underset{\sim}{\varepsilon}^e}, \quad \eta = -\frac{\partial\psi}{\partial T}, \quad R = -\rho\frac{\partial\psi}{\partial\alpha} \quad a = \rho\frac{\partial\psi}{\partial p_\chi}, \quad \underline{b} = \rho\frac{\partial\psi}{\partial\nabla p_\chi} \qquad (16.14)$$

and the residual dissipation is

$$D^{res} = \underset{\sim}{\sigma} : \dot{\underset{\sim}{\varepsilon}}^p + R\dot{\alpha} - \frac{q}{T}.\nabla T \geq 0 \qquad (16.15)$$

where R is the thermodynamic force associated with the internal variable α. The existence of a convex dissipation potential, $\Omega(\underset{\sim}{\sigma}, R)$ depending on the thermodynamic forces can then be assumed from which the evolution rules for internal variables are derived, that identically fulfil the entropy inequality, as usually done in classical continuum thermomechanics (Germain et al, 1983):

$$\dot{\underset{\sim}{\varepsilon}}^p = \frac{\partial \Omega}{\partial \underset{\sim}{\sigma}}, \quad \dot{\alpha} = \frac{\partial \Omega}{\partial R} \tag{16.16}$$

After presenting the general approach, we readily give the most simple example which provides a direct connection to several existing generalized continuum models. The free energy density function ψ is chosen as a function of the generalized relative strain variable e defined as:

$$e = p - p_\chi \tag{16.17}$$

where p is the cumulative plastic strain, thus introducing a coupling between macro and micromorphic plastic variables. Assuming isotropic material behaviour for brevity, the additional contributions to the free energy are taken as quadratic functions of e and ∇p_χ:

$$\psi(\underset{\sim}{\varepsilon}^e, T, \alpha, p_\chi, \nabla p_\chi) = \psi^{(1)}(\underset{\sim}{\varepsilon}^e, T, \alpha) + \frac{1}{2} H_\chi (p - p_\chi)^2 + \frac{1}{2} A \nabla p_\chi \cdot \nabla p_\chi \tag{16.18}$$

where H_χ and A are the additional moduli introduced by the micrmorphic model. The function $\psi^{(1)}(\underset{\sim}{\varepsilon}^e, T, \alpha)$ refers to any constitutive function in a classical continuum thermomechanical model with internal variables. After inserting the state laws (16.14)

$$a = \rho \frac{\partial \psi}{\partial p_\chi} = -H_\chi (p - p_\chi), \quad \underset{\sim}{b} = \rho \frac{\partial \psi}{\partial \nabla p_\chi} = A \nabla p_\chi \tag{16.19}$$

into the additional balance equation (16.8), the following partial differential equation for p_χ is obtained, at least for a homogeneous material under isothermal conditions:

$$p = p_\chi - \frac{A}{H_\chi} \Delta p_\chi \tag{16.20}$$

where Δ is the Laplace operator. It involves a characteristic length scale defined by:

$$l_c^2 = \frac{A}{H_\chi} \tag{16.21}$$

The additional material parameters H_χ and A are assumed to be positive in this work. This does not exclude a softening material behaviour that can be induced by the proper evolution of the internal variables.

Let us now choose a yield function in the form

$$f(\underset{\sim}{\sigma}, R) = \sigma_{eq} - \sigma_Y - R \tag{16.22}$$

where σ_{eq} is an equivalent stress measure, σ_Y the initial yield stress and $R(p)$ is here the hardening (or softening) function. It follows from the state law (16.14) and from the balance equation (16.20) that

$$R = \frac{\partial \psi}{\partial p} = R(p) + H_\chi (p - p_\chi) = R(p) - A \Delta p_\chi \tag{16.23}$$

which shows the enhanced hardening due to the plastic microstrain. Under plastic loading condition,

$$\sigma_{eq} = \sigma_Y + R(p) - A\Delta p_\chi \tag{16.24}$$

which is reminiscent of Aifantis celebrated strain gradient plasticity model (Aifantis, 1984). The equivalence with Aifantis model is obtained for $H_\chi = \infty$ which enforces the internal constraint: $p_\chi \simeq p$.

16.2.2 Direct Construction of Gradient Plasticity Theory

The method of virtual power can also be used directly to construct the strain gradient plasticity model without resorting to the micromorphic model (Forest and Bertram, 2011). The enriched power density of internal forces and of contact forces are introduced as

$$p^{(i)} = \underset{\sim}{\sigma} : \dot{\underset{\sim}{\varepsilon}} + a\dot{p} + \underline{b} \cdot \nabla\dot{p}, \quad p^{(c)} = \underline{t} \cdot \dot{\underline{u}} + a^c\dot{p} \tag{16.25}$$

where a and $\underline{b}$ are generalized stresses acting on the virtual plastic field $\dot{p}$ and its gradient, respectively. The usual traction vector is $\underline{t}$ and a^c denotes the generalized traction. Such generalized stresses are called micro–forces by Gurtin (2003). A generalized principle of virtual power is stated with respect to the virtual fields of displacements and the p–variable. The application of this principle results in the same balance equations and boundary conditions as in Eq. (16.7) to (16.9).

The constitutive functions now depend on cumulative plastic strain and its gradient. The Clausius–Duhem inequality then becomes:

$$(\underset{\sim}{\sigma} - \rho\frac{\partial\psi}{\partial\underset{\sim}{\varepsilon}^e}) : \dot{\underset{\sim}{\varepsilon}}^e + (a - \rho\frac{\partial\psi}{\partial p})\dot{p} + (\underline{b} - \rho\frac{\partial\psi}{\partial\nabla p}) \cdot \nabla\dot{p} + \underset{\sim}{\sigma} : \dot{\underset{\sim}{\varepsilon}}^p \geq 0 \tag{16.26}$$

At this stage, the following state laws are adopted

$$\underset{\sim}{\sigma} = \rho\frac{\partial\psi}{\partial\underset{\sim}{\varepsilon}^e}, \quad a = \rho\frac{\partial\psi}{\partial p} + R, \quad \underline{b} = \rho\frac{\partial\psi}{\partial\nabla p} \tag{16.27}$$

thus assuming that no dissipation is associated with the generalized stress $\underline{b}$. This is the most simple assumption that is sufficient for deriving Aifantis model, in particular. The residual dissipation is then

$$\underset{\sim}{\sigma} : \dot{\underset{\sim}{\varepsilon}}^p + R\dot{p} \geq 0 \tag{16.28}$$

A simple quadratic free energy potential is chosen

$$\rho\psi(\underset{\sim}{\varepsilon}^e, p, \nabla p) = \frac{1}{2}\underset{\sim}{\varepsilon}^e : \underset{\sim}{C} : \underset{\sim}{\varepsilon}^e + \frac{1}{2}Hp^2 + \frac{1}{2}A\nabla p \cdot \nabla p \tag{16.29}$$

from which the state laws are derived:

$$\sigma = \underset{\sim}{C} : \underset{\sim}{\varepsilon}^e, \quad R = -Hp + a, \quad \underline{b} = A\nabla p \tag{16.30}$$

where $\underset{\sim}{C}$ is the four–rank tensor of the elastic moduli, H is the usual hardening modulus and A is an additional material parameter (unit MPa·mm^2). The yield function is taken as

$$f(\underset{\sim}{\sigma}, R) = \sigma_{eq} - \sigma_Y + R \tag{16.31}$$

Under plastic loading, this gives

$$\sigma_{eq} = \sigma_Y - R = \sigma_Y + Hp - a = \sigma_Y + Hp - \operatorname{div} \underline{b} = \sigma_Y + Hp - A\nabla^2 p \tag{16.32}$$

which is Aifantis celebrated equation, to be compared with Eq. (16.24). The plasticity flow and evolution rules are

$$\dot{\underset{\sim}{\varepsilon}}^p = \lambda \frac{\partial f}{\partial \underset{\sim}{\sigma}}, \quad \dot{p} = \lambda \frac{\partial f}{\partial R} = \lambda \tag{16.33}$$

in the rate–independent case, λ being the plastic multiplier.

The enhanced power of internal forces has been used also by Gurtin and Anand (2009) for gradient plasticity and by Frémond and Nedjar (1996) for gradient damage. However, there exist alternative formulations avoiding the modification of $p^{(i)}$, see Nguyen (2010b, 2016).

16.3 Gradient of Entropy or Temperature Models

It was shown in the previous section that the free energy function can depend on the gradient of strain or on any internal variable like plastic strain and damage. This requires an amendment of the principle of virtual power with the introduction of generalized stress tensors. A similar question arises in the case of heat transfer: can the free energy function depend on the temperature gradient? In the standard continuum thermodynamics framework, the answer is no (Coleman and Mizel, 1963). However, this impossibility can be overcome by suitable enhancement of the theoretical framework. Several tracks have been proposed in the literature for that purpose which are reviewed in Liu et al (2017) with special consideration of the consequences on the heat equations.

In this part, the mechanical contributions are omitted for the sake of conciseness.

16.3.1 A Principle of Virtual Power for Entropy

One track is presented here based on the formulation of a principle of virtual power for entropy (or temperature) and its gradient following (Forest and Amestoy, 2008).

It is postulated that the entropy rate and its gradient contribute to the power of internal and external forces, in the form:

$$\mathscr{P}^{(i)}(\dot{\eta}^{\star}) = -\int_{\mathscr{D}} (a_{\eta}\dot{\eta}^{\star} + \underline{b}_{\eta} \cdot \nabla\dot{\eta}^{\star})\, dV \qquad (16.34)$$

$$\mathscr{P}^{(e)}(\dot{\eta}^{\star}) = \int_{\mathscr{D}} (a_{\eta}^{p}\dot{\eta}^{\star} + \underline{b}_{\eta}^{p} \cdot \nabla\dot{\eta}^{\star})\, dV + \int_{\partial\mathscr{D}} a_{\eta}^{c}\dot{\eta}^{\star}\, dS \qquad (16.35)$$

in addition to the purely mechanical parts not recalled here, where $\dot{\eta}^{\star}$ is a field of virtual rate of change of entropy density. These power densities involve internal scalar and vector generalized stresses a_{η}, $\underline{b}_{\eta}$, on the one hand, and prescribed external scalar and vector volume microforces a_{η}^{p}, $\underline{b}_{\eta}^{p}$ and a generalized surface traction a_{η}^{c}, on the other hand.

The exploitation of the principle of virtual power with respect to the virtual field $\dot{\eta}^{\star}$ results in the following independent variational equation:

$$\mathscr{P}^{(i)}(\dot{\eta}^{\star}) + \mathscr{P}^{(e)}(\dot{\eta}^{\star}) = 0, \quad \forall\mathscr{D} \subset \mathscr{B}, \quad \forall\dot{\eta}^{\star} \qquad (16.36)$$

provided that no "microinertia" effects are attached to variable η (Svendsen, 1999). Such terms involving the second derivative of temperature or entropy can be introduced following (Liu et al, 2017). It is used to derive a balance equation associated with variable η and the associated boundary condition:

$$\mathrm{div}\,(\underline{b}_{\eta} - \underline{b}_{\eta}^{p}) - a_{\eta} + a_{\eta}^{p} = 0, \quad \forall\underline{x} \in \mathscr{D}, \quad a_{\eta}^{c} = (\underline{b}_{\eta} - \underline{b}_{\eta}^{p})\cdot\underline{n}, \quad \forall\underline{x} \in \partial\mathscr{D} \qquad (16.37)$$

It is essential that the power of external forces $(16.35)_2$ contributes to the global balance of energy:

$$\dot{\mathscr{E}} = \int_{\mathscr{D}} \rho\dot{e}\, dV = \mathscr{P}^{(e)}(\dot{\eta}) - \int_{\partial\mathscr{D}} \underline{q} \cdot \underline{n}\, dS \qquad (16.38)$$

An alternative form is obtained after taking the generalized principle of virtual power into account:

$$\dot{\mathscr{E}} = -\mathscr{P}^{(i)}(\dot{\eta}) - \int_{\partial\mathscr{D}} \underline{q} \cdot \underline{n}\, dS \qquad (16.39)$$

The local form of energy balance follows:

$$\rho\dot{e} = a_{\eta}\dot{\eta} + \underline{b}_{\eta} \cdot \nabla\dot{\eta} - \mathrm{div}\,\underline{q} \qquad (16.40)$$

The entropy principle is assumed to keep its classical global form, for any material subdomain $\mathscr{D} \subset \mathscr{B}$:

$$\frac{d}{dt}\int_{\mathscr{D}} \rho\eta\, dV \geq -\int_{\partial\mathscr{D}} \frac{\underline{q}}{T}\, dS \qquad (16.41)$$

The additional contributions appear in the generalized Clausius–Duhem inequality:

$$\rho(T\dot{\eta} - \dot{\epsilon}) + a_\eta \dot{\eta} + \underline{b}_\eta \cdot \nabla\dot{\eta} - \frac{q}{T} \cdot \nabla T \geq 0 \qquad (16.42)$$

The constitutive functions of solids of this kind depend on the set of state variables $(\eta, \nabla\eta)$. After inserting these dependencies, the Clausius–Duhem inequality (16.42) becomes:

$$\rho(T - \frac{\partial\epsilon}{\partial\eta} + \frac{a_\eta}{\rho})\dot{\eta} + (\underline{b}_\eta - \rho\frac{\partial\epsilon}{\partial\nabla\eta}) \cdot \nabla\dot{\eta} - \frac{q}{T} \cdot \nabla T \geq 0 \qquad (16.43)$$

from which the state laws are derived,

$$T = \frac{\partial\epsilon}{\partial\eta} - \frac{a_\eta}{\rho}, \quad \underline{b}_\eta = \rho\frac{\partial\epsilon}{\partial\nabla\eta} \qquad (16.44)$$

Accordingly, the temperature is found to be equal to the partial derivative of the internal energy function with respect to entropy complemented by a contribution of the internal scalar microstress a_η. The internal generalized stress vector $\underline{b}_\eta$ is nothing but the partial derivative of internal energy with respect to the entropy gradient. It is called the hypertemperature vector (Forest and Amestoy, 2008). The residual dissipation reduces to:

$$-\frac{q}{T} \cdot \nabla T \geq 0 \qquad (16.45)$$

First consequences of the additional or modified state laws established previously are investigated in the simplest case, namely that of the rigid heat conductor. After inserting the state laws (16.44) into the local energy balance (16.40), the following usual form of the heat equation is recovered:

$$\rho T\dot{\eta} = -\text{div}\,\underline{q} \qquad (16.46)$$

In the sequel, a specific constitutive function for internal energy is chosen for the illustration of the modifications brought in the governing equations of thermal conduction by the introduction of entropy gradient effects. A specific constitutive relation will also be needed for the heat flux vector in order to obtain an explicit partial differential equation for entropy. In the present theory, there is no need for departing from the classical Fourier law of heat conduction:

$$\underline{q} = -\kappa\nabla T \qquad (16.47)$$

written here for isotropic materials for simplicity. So in the present theory, heat still flows from hot to cold and there is no up–hill heat diffusion.

The explicit heat equation associated with the gradient of entropy theory is now derived for isotropic materials. We take $a_\eta^p = 0$ and $\underline{b}_\eta^p = 0$ for the sake of brevity. Material homogeneity is also assumed for simplicity. The mass density ρ is constant and homogeneous.

The expression of the internal energy density function in a rigid heat conducting body is linearised around the reference entropy value η_0. According to the gradient of entropy model, it contains quadratic terms in the entropy and entropy gradient:

$$\rho\epsilon(\eta,\nabla\eta) = \rho\eta T_0 + \frac{\rho^2(\eta-\eta_0)^2}{4\beta} + \frac{1}{2}A_\eta\nabla\eta\cdot\nabla\eta \tag{16.48}$$

where β and A_η are (strictly positive) material parameters. The expression of the generalized stresses are derived from the additional state and balance laws:

$$\underline{b}_\eta = \rho\frac{\partial\epsilon}{\partial\nabla\eta} = A_\eta\nabla\eta, \quad a_\eta = \mathrm{div}\,\underline{b}_\eta = A_\eta\Delta\eta \tag{16.49}$$

where Δ is the Laplace operator. Compared to classical linearised thermal diffusion, the temperature function is modified as follows:

$$T = \frac{\partial\epsilon}{\partial\eta} - \frac{a_\eta}{\rho} = T_0 + \frac{\rho(\eta-\eta_0)}{2\beta} - \frac{A_\eta}{\rho}\Delta\eta \tag{16.50}$$

Keeping the usual form (16.47) of Fourier heat conduction law, the heat equation can now be derived as

$$\rho T_0\dot{\eta} = \frac{\rho\kappa}{2\beta}(\Delta\eta - l_\eta^2\Delta^2\eta), \quad \text{with} \quad l_\eta^2 = \frac{2\beta A_\eta}{\rho^2} \tag{16.51}$$

This enhanced heat equation has the structure of the Cahn–Hilliard equation in mass transport theory as derived in Cahn and Hilliard (1958); Gurtin (1996). It involves a characteristic (positive) length l_η related to material parameters. The classical heat equation is retrieved for a vanishing intrinsic length scale $l_\eta = 0$, or equivalently $A_\eta = 0$, in the absence of prescribed external microforces.

16.3.2 Gradient of Entropy or Gradient of Temperature?

The initial question raised in this part was the introduction of the temperature gradient in the free energy density function. The previous theory was developed for the entropy gradient instead. This is due to the fact that the first function of state in thermodynamics is the internal energy density which is a function of entropy and strain in general. The question of the introduction of a gradient term must therefore be asked first at this stage. A similar construction as before is possible for a gradient of temperature theory. It was shown in Forest and Amestoy (2008) to deliver a distinct theory from the gradient of entropy one. The gradient of temperature and gradient of entropy models are not dual contrary to the usual case where the entropy based and temperature based theories are dual in the absence of gradients. The same situation is encountered in mechanics where the strain gradient theory and the recently proposed stress gradient model are no dual theories (Forest and Sab, 2012, 2017).

Alternative formulations of the gradient of temperature models were proposed in Ireman and Nguyen (2004); Nguyen (2010a,b) without resorting to additional power contributions but, instead, by modifying the definition of the free energy function and extending the concept of standard generalized materials to the gradient case.

They lead to heat equations that differ from Eq. (16.51) and that possibly include the possibility of heat wave propagation.

The method of virtual power can be used to propose new theories of heat conductors including microtemperature or microentropy concepts (Forest and Aifantis, 2010). The predicted effects are similar to those deduced from double temperature models where each material point is characterized by two distinct temperatures, similarly to mixture theory for fluids.

16.4 The Method of Virtual Power Applied to Phase Field Modelling

The phase field variable ϕ usually is an order parameter with continuous values ranging from 0 to 1. It very often serves as a phase indicator in combination with a concentration field, c, of some solute species in solid body (Finel et al, 2010). Virtual fields of order parameter $\phi^\star$ are considered with suitable regularity[1]. The virtual power of internal generalized forces is defined by the integral over the volume $\mathscr{D} \subset \mathscr{B}$ of a power density, which is assumed *a priori* to be a linear form represented by the generalized stress measures a and $\underline{b}$ (Ammar et al, 2009):

$$\mathscr{P}^{(i)}(\phi^\star, \mathscr{D}) = -\int_{\mathscr{D}} (a\phi^\star + \underline{b} \cdot \nabla\phi^\star) \, dV$$

$$= -\int_{\mathscr{D}} (a - \nabla \cdot \underline{b}) \phi^\star \, dV - \int_{\partial\mathscr{D}} (\underline{b} \cdot \underline{n}) \phi^\star \, dS \qquad (16.52)$$

The next step is to introduce the virtual power of external forces applied to the considered body. It can be split into a virtual power density of long range volume forces, which can include, in general, a volume density of scalar external generalized forces γ and vector external generalized force $\underline{\gamma}$:

$$\mathscr{P}^{(e)}(\phi^\star, \mathscr{D}) = \int_{\mathscr{D}} (\gamma\phi^\star + \underline{\gamma} \cdot \nabla\phi^\star) \, dV$$

$$= \int_{\mathscr{D}} (\gamma - \nabla \cdot \underline{\gamma}) \phi^\star \, dV + \int_{\partial\mathscr{D}} (\underline{\gamma} \cdot \underline{n}) \phi^\star \, dS \qquad (16.53)$$

and a virtual power density of generalized contact forces, represented by a surface density a^c of generalized traction:

$$\mathscr{P}^{(c)}(\phi^\star, \mathscr{D}) = \int_{\partial\mathscr{D}} a^c \phi^\star \, dS \qquad (16.54)$$

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[1] In fact, as in distribution theory, it is sufficient to take them as differentiable at any order with compact support.

A possible power of inertial microforces is not envisaged here. According to the principle of virtual power, the total virtual power of all forces vanishes on any subdomain $\mathscr{D} \subset \mathscr{B}$ and for any virtual order parameter field $\phi^\star$:

$$\mathscr{P}^{(i)}(\phi^\star, \mathscr{D}) + \mathscr{P}^{(c)}(\phi^\star, \mathscr{D}) + \mathscr{P}^{(e)}(\phi^\star, \mathscr{D}) = 0, \quad \forall \phi^\star, \forall \mathscr{D} \subset \mathscr{B} \qquad (16.55)$$

$$\int_{\mathscr{D}} (-a + \nabla \cdot \underline{b} + \gamma - \nabla \cdot \underline{\gamma}) \phi^\star \, dV + \int_{\partial\mathscr{D}} (a^c - \underline{b} \cdot \underline{n} + \underline{\gamma} \cdot \underline{n}) \phi^\star \, dS = 0 \qquad (16.56)$$

This identity can be satisfied for any field $\phi^\star$ and $\forall \mathscr{D}$ if and only if:

$$a - \nabla \cdot (\underline{b} - \underline{\gamma}) - \gamma = 0 \quad \text{in} \quad \mathscr{B}, \qquad a^c = (\underline{b} - \underline{\gamma}) \cdot \underline{n} \quad \text{on} \quad \partial\mathscr{B} \qquad (16.57)$$

Equation $(16.57)_1$ expresses the general form of balance of generalized stresses. It is identical with Gurtin's balance of microforces (Gurtin, 1996), except the external microforce contribution γ that may exist in general. In the sequel, however, it is assumed that $\gamma = 0$ and $\underline{\gamma} = 0$ for the sake of brevity. The equation $(16.57)_2$ represents the boundary condition for the generalized traction vector.

State Laws and Dissipation Potential

According to the first principle of thermodynamics, the time variation of the total energy in a material subdomain is equal to the power of external forces acting on it. In the absence of inertial forces, the total energy is reduced to the internal energy with density e. Then, the energy balance is stated as:

$$\int_{\mathscr{D}} \dot{e} \, dV = \mathscr{P}^{(e)} + \mathscr{P}^{(c)} = -\mathscr{P}^{(i)} = \int_{\mathscr{D}} a\dot{\phi} + \underline{b} \cdot \nabla\dot{\phi} \, dV \qquad (16.58)$$

This identity is valid for any subdomain $\mathscr{D} \subset \mathscr{B}$. The local form of the energy balance is obtained:

$$\dot{e} = a\dot{\phi} + \underline{b} \cdot \nabla\dot{\phi} = \nabla \cdot (\dot{\phi}\underline{b}) \qquad (16.59)$$

The entropy principle is formulated as follows:

$$\int_{\mathscr{D}} \dot{\eta} \, dV \geq -\int_{\partial\mathscr{D}} \underline{\Phi} \cdot \underline{n} \, dS \quad \text{and} \quad \underline{\Phi} = -\mu \frac{\underline{J}}{T} \qquad (16.60)$$

where η is the entropy density, $\underline{\Phi}$ the entropy flux, $\underline{J}$ the diffusion flux and μ the diffusion potential (Villani et al, 2014). Using the equation of local conservation of mass:

$$\dot{c} = -\nabla \cdot \underline{J} \qquad (16.61)$$

the following local form of the entropy inequality is obtained:

$$T\dot{\eta} - \nabla \cdot (\mu \underline{J}) \geq 0 \tag{16.62}$$

Combining the equation of the free energy density $\psi = \dot{\epsilon} - T\dot{\eta}$ in the isothermal case with Eqs. (16.59)–(16.62), leads to the Clausius-Duhem inequality:

$$-\dot{\psi} + a\dot{\phi} + \underline{b} \cdot \nabla\dot{\phi} - \underline{J} \cdot \nabla\mu - \mu\nabla \cdot \underline{J} \geq 0 \tag{16.63}$$

The free energy density is assumed to be a function of concentration c, order parameter ϕ, as well as its gradient $\nabla\phi$. The Clausius-Duhem inequality can then be written as follows:

$$\left(\mu - \frac{\partial\psi}{\partial c}\right)\dot{c} + \left(a - \frac{\partial\psi}{\partial\phi}\right)\dot{\phi} + \left(\underline{b} - \frac{\partial\psi}{\partial\nabla\phi}\right) \cdot \nabla\dot{\phi} - \underline{J} \cdot \nabla\mu \geq 0 \tag{16.64}$$

For every admissible process and for any given $(c, \phi, \nabla\phi)$, the inequality (16.64) must hold for arbitrary values of $\dot{c}$, $\dot{\phi}$ and $\nabla\dot{\phi}$. The microstress $\underline{b}(c, \phi, \nabla\phi)$ and the diffusion potential $\mu(c, \phi, \nabla\phi)$ are assumed independent of $\nabla\dot{\phi}$ and $\dot{c}$. The following state laws are deduced:

$$\mu = \frac{\partial\psi}{\partial c}, \quad \underline{b} = \frac{\partial f}{\partial\nabla\phi} = A\nabla\phi \tag{16.65}$$

the latter equation being valid in the case of a quadratic potential w.r.t. $\nabla\phi$. The Clausius-Duhem inequality then reduces to the residual dissipation:

$$D = -\underline{J} \cdot \nabla\mu + a^{dis}\dot{\phi} \geq 0 \quad \text{with} \quad a^{dis} = a - \frac{\partial\psi}{\partial\phi} \tag{16.66}$$

where a^{dis} is the chemical force associated with the dissipative processes, as introduced in Gurtin (1996).

In order to define the complementary laws related to the dissipative processes, the existence of a dissipation potential function $\Omega(\nabla\mu, \pi_{dis})$ is assumed. The retained specific form is the following:

$$\Omega(\nabla\mu, a^{dis}) = \frac{1}{2}L(\phi)\nabla\mu \cdot \nabla\mu + \frac{1}{2\beta}a^{dis2} \tag{16.67}$$

where $L(\phi)$ and β are material parameters or functions.

The complementary evolution laws derive from the dissipation potential:

$$\dot{\phi} = \frac{\partial\Omega}{\partial a^{dis}} = \frac{1}{\beta}a^{dis}, \quad \underline{J} = -\frac{\partial\Omega}{\partial\nabla\mu} = -L(\phi)\nabla\mu \tag{16.68}$$

The convexity of the dissipation potential ensures the positivity of dissipation.

Combining Eqs. (16.66) and (16.68), one gets:

$$a = \beta\,\dot{\phi} + \frac{\partial\psi}{\partial\phi} \tag{16.69}$$

The substitution of the two state laws and the complementary laws, into the balance equations for mass concentration and generalized stresses respectively leads to the evolution equations for concentration and order parameter:

$$\dot{c} = -\nabla\cdot(-L(\phi)\nabla\mu) = -\nabla\cdot\left(-L(\phi)\nabla\frac{\partial\psi}{\partial c}\right) \tag{16.70}$$

$$a - \nabla\cdot\underline{b} = \beta\dot{\phi} - \alpha\Delta\phi + \frac{\partial\psi}{\partial\phi} = 0 \tag{16.71}$$

The usual diffusion and Cahn–Allen / Ginzburg–Landau equations are thus retrieved (Finel et al, 2010).

In the previous theory, the free energy density depends on the gradient of the order parameter but not on the concentration gradient. This possibility is investigated in the next section.

16.5 On the Construction of the Cahn–Hilliard Diffusion Theory

The partial differential equation for the concentration field according to Cahn and Hilliard (1958) is the following

$$\dot{c} = \kappa\Delta\left(\frac{\partial\psi}{\partial c} - A\Delta c\right) \tag{16.72}$$

with the special case: $\dot{c} = \beta\nabla^2 c - \chi\nabla^4 c$ when the free energy potential is quadratic w.r.t. c and ∇c. We present in this section three distinct derivations of these field equations from first principles. The first one was initially proposed by Cahn and Hilliard. The second one is based on the principle of virtual power with an additional generalized balance equation, following Gurtin (1996). In the last subsection, a variational formulation is proposed considering a second gradient theory of diffusion.

16.5.1 Usual Presentation Based on the Variational Derivative

A homogeneous material system is considered with composition c of a given solute element. The free energy density $\psi(c,\nabla c)$ is assumed to depend not only on concentration but also on its gradient, as initially proposed by Cahn and Hilliard (1958):

$$F = \int_{\mathscr{B}} \psi \, dV = \int_{\mathscr{B}} \left(\psi_0(c) + \kappa_1 \nabla^2 c + \kappa_2 (\nabla c) \cdot (\nabla c) \right) dV$$

$$= \int_{\mathscr{B}} \left(\psi_0(c) + \frac{1}{2} A (\nabla c) \cdot (\nabla c) \right) dV \tag{16.73}$$

in the isotropic case. The second expression holds assuming $(\nabla c) \cdot \underline{n} = 0$ on $\partial\mathscr{B}$. The potential $\psi_0(c)$ is the usual potential depending on concentration in classical diffusion theory. The variational derivative of the total free energy of the body is defined as

$$\delta F = \int_{\mathscr{B}} \delta \psi \, dV = \int_{\mathscr{B}} \left(\frac{\partial \psi}{\partial c} \delta c + \frac{\partial \psi}{\partial \nabla c} \delta \nabla c \right) dV \tag{16.74}$$

Note that $\nabla \cdot (\delta c \nabla c) = \nabla c \cdot \delta \nabla c + \delta c \Delta c$ so that

$$\int_{\mathscr{B}} \nabla \cdot (\delta c \nabla c) \, dV = \int_{\partial\mathscr{B}} \delta c \nabla c \cdot \underline{n} \, dS = 0, \quad \text{if} \quad \nabla c \cdot \underline{n} = 0 \text{ on } \partial\mathscr{B}$$

$$= \int_{\mathscr{B}} \nabla c \cdot \delta \nabla c \, dV + \int_{\mathscr{B}} \delta c \Delta c \, dV \tag{16.75}$$

Hence

$$\delta F = \int_{\mathscr{B}} \left(\frac{\partial \psi_0}{\partial c} - A \Delta c \right) \delta c \, dV \tag{16.76}$$

The variational derivative of the free energy function then is

$$\frac{\delta \psi}{\delta c} := \frac{\partial \psi_0}{\partial c} - A \Delta c \tag{16.77}$$

which makes sense only in the absence diffusion flux $\nabla c \cdot \underline{n}$ on the boundary of the body or in periodic systems. The balance of mass and Fick's law for the mass flux write

$$\dot{c} = -\nabla \cdot \underline{J}, \quad \underline{J} = -\kappa \nabla \mu \tag{16.78}$$

The diffusion potential μ is defined as the variational derivative of the free energy density function:

$$\mu := \frac{\delta \psi}{\delta c} \tag{16.79}$$

The combination of mass balance, Fick's law and constitutive potential ψ leads to the Cahn-Hilliard equation:

$$\dot{c} = \nabla \cdot \left(\kappa \nabla \frac{\delta \psi}{\delta c} \right) = \kappa \Delta \frac{\delta \psi}{\delta c} = \kappa \Delta \left(\frac{\partial \psi_0}{\partial c} - A \Delta c \right) \tag{16.80}$$

This is the general form for a conserved quantity in contrast to non–conserved phase field or order parameter considered in the previous section.

16.5.2 Method of Virtual Power with Additional Balance Equation

The existence of a principle of virtual power w.r.t. to the concentration field and its gradient is assumed. The power density of generalized internal and contact forces is

$$p^{(i)} = a\dot{c} + \underline{b} \cdot \nabla \dot{c}, \quad p^{(c)} = a^c \dot{c} \tag{16.81}$$

This leads to a field equation for the balance of generalized forces a and $\underline{b}$, and associated boundary conditions:

$$a = \text{div}\,\underline{b}, \quad \underline{b} \cdot \underline{n} = a^c \tag{16.82}$$

in addition to the balance of mass $\dot{c} = -\text{div}\,\underline{J}$. The first and second principles (isothermal case) take the form

$$\dot{\epsilon} = p^{(i)}, \quad -\dot{\psi} + p^{(i)} - \text{div}\,(\mu\underline{J}) \geq 0 \tag{16.83}$$

It should be noted that in the absence of concentration gradient in the free energy potential, the generalized forces a and $\underline{b}$ identically vanish and the classical diffusion theory is retrieved, as it should. The Clausius-Duhem inequality is

$$\left(a + \mu - \frac{\partial \psi}{\partial c}\right)\dot{c} + \left(\underline{b} - \frac{\partial \psi}{\partial \nabla c}\right) \cdot \nabla \dot{c} - \underline{J} \cdot \nabla \mu \geq 0 \tag{16.84}$$

leading to the state laws

$$\mu = \frac{\partial \psi}{\partial c} - a, \quad \underline{b} = \frac{\partial \psi}{\partial \nabla c} \tag{16.85}$$

Fick's law (16.78) and the potential (16.73) are used again. The Cahn–Hilliard equations are now obtained by combining the balance and constitutive equations in the following way:

$$\mu = \frac{\partial \psi}{\partial c} - a = \frac{\partial \psi}{\partial c} - \text{div}\,\underline{b} = \frac{\partial \psi}{\partial c} - A\Delta c, \tag{16.86}$$

$$\dot{c} = -\text{div}\,\underline{J} = \kappa\Delta\mu = \kappa\Delta\left(\frac{\partial \psi}{\partial c} - A\Delta c\right) \tag{16.87}$$

The Cahn–Hilliard model can also be derived from a more general theory introducing micromorphic concentration or microconcentration variables c_χ and its gradient in addition to the concentration as done in Sect. 16.3 for the entropy or temperature. The internal constraint $c \equiv c_\chi$ leads to the previous equations (Forest, 2008). The microconcentration can be regarded as a description of the variance of the composition inside the volume element.

16.5.3 Second Gradient Diffusion Theory

The Cahn–Hilliard equations can also be interpreted as emerging from a second
gradient theory of diffusion. For that purpose, let us first recall the

16.5.3.1 Variational Formulation of Classical Diffusion

The variational formulation of the field and boundary equations of classical diffusion,
namely

$$-\nabla \cdot \underline{J} + \gamma = \dot{c} \quad \text{on} \quad \mathscr{B}, \qquad j = \underline{J} \cdot \underline{n} \quad \text{on} \quad \partial \mathscr{B} \tag{16.88}$$

can be written in the form $\forall c^\star, \forall \mathscr{D} \subset \mathscr{B}$

$$\mathscr{I}^{(i)}(c^\star, \mathscr{D}) + \mathscr{I}^{(c)}(c^\star, \mathscr{D}) + \mathscr{I}^{(e)}(c^\star, \mathscr{D}) + \mathscr{I}^{(a)}(c^\star, \mathscr{D)} = 0 \tag{16.89}$$

for test compositions $c^\star$ and with the following contributions

$$\mathscr{I}^{(i)}(c^\star, \mathscr{D}) = \int_{\mathscr{D}} \underline{J} \cdot \nabla c^\star \, dV, \quad \mathscr{I}^{(c)}(c^\star, \mathscr{D}) = -\int_{\partial \mathscr{D}} jc^\star \, dS \tag{16.90}$$

$$\mathscr{I}^{(e)}(c^\star, \mathscr{D}) = \int_{\mathscr{D}} \gamma c^\star \, dV, \quad \mathscr{I}^{(a)}(c^\star, \mathscr{D}) = -\int_{\mathscr{D}} \dot{c} c^\star \, dV \tag{16.91}$$

In other words,

$$\int_{\mathscr{D}} (-\nabla \cdot \underline{J} + \gamma - \dot{c}) c^\star \, dV + \int_{\partial \mathscr{D}} (\underline{J} \cdot \underline{n} - j) c^\star \, dS = 0 \tag{16.92}$$

16.5.3.2 Variational Formulation of Second Gradient Diffusion

The internal contribution (16.90) is extended by introducing the second gradient of
the test functions and a generalized second order flux tensor:

$$\mathscr{I}^{(i)}(c^\star, \mathscr{D}) = \int_{\mathscr{D}} \left(\underline{J} \cdot \nabla c^\star + \underset{\sim}{K} : \nabla \nabla c^\star \right) dV \tag{16.93}$$

Two integration by parts are necessary to obtain the form of the generalized surface
flux:

$$\mathscr{I}^{(i)}(c^\star, \mathscr{D}) = \int_{\mathscr{D}} \left((J_i c^\star)_{,i} + (K_{ij}c^\star_{,i})_{,j} - J_{i,i}c^\star - K_{ij,j}c^\star_{,i} \right) dV$$

$$= \int_{\mathscr{D}} \left((J_i c^\star)_{,i} + (K_{ij}c^\star_{,i})_{,j} - J_{i,i}c^\star - (K_{ij,j}c^\star)_{,i} + K_{ij,ij}c^\star \right) dV$$

$$= \int_{\partial\mathscr{D}} \left(J_i c^\star + K_{ij}c^\star_{,i} - K_{ij,j}c^\star \right) n_i\, dS - \int_{\mathscr{D}} (J_{i,i} - K_{ij,ij})c^\star\, dV$$

$$= \int_{\partial\mathscr{D}} \left(\underline{J} - \underset{\sim}{K}\cdot\nabla \right)\cdot\underline{n}\, c^\star\, dS + \int_{\partial V} (\underset{\sim}{K}\cdot\underline{n})\cdot\nabla c^\star\, dS - \int_V ((\underline{J} - \underset{\sim}{K}\cdot\nabla)\cdot\nabla)c^\star\, dV$$

At this stage, tangent and normal derivatives, $\underline{D}_t$ and D_n of the concentration field on surfaces must be distinguished:

$$\nabla c = \underline{D}_t c + (D_n c)\underline{n}, \quad D_n c = \nabla c \cdot \underline{n} \tag{16.94}$$

It follows that

$$\int_{\partial\mathscr{D}} (\underset{\sim}{K}\cdot\underline{n})\cdot\nabla c^\star\, dS = \int_{\partial\mathscr{D}} (\underset{\sim}{K}\cdot\underline{n})\cdot\underline{D}_t c^\star\, dS + \int_{\partial\mathscr{D}} (\underline{n}\cdot\underset{\sim}{K}\cdot\underline{n})D_n c^\star\, dS \tag{16.95}$$

An integration by parts of the integral involving the tangent derivative is possible:

$$\int_{\partial\mathscr{D}} (\underset{\sim}{K}\cdot\underline{n})\cdot\underline{D}_t c^\star\, dS = \int_{\partial\mathscr{D}} \underline{D}_t\cdot(\underset{\sim}{K}\cdot\underline{n}\,c^\star)\, dS - \int_{\partial\mathscr{D}} (\underline{D}_t\cdot(\underset{\sim}{K}\cdot\underline{n}))c^\star\, dS \tag{16.96}$$

The divergence theorem for surfaces[2] can be applied to the first term of the right-hand side to get the final expression of

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[2] The divergence theorem for a closed and smooth surface ∂V (no edge) is

$$\int_{\partial V} \underline{D}_t\cdot\underline{q}\, dS = \int_{\partial V} 2\mathscr{C}\,\underline{q}\cdot\underline{n}\, dS, \quad \text{with} \quad 2\mathscr{C} = \underline{D}_t\cdot\underline{n}$$

where $\mathscr{C}$ is the mean local curvature.

Proof. Evaluate

$$\underline{\text{curl}}\,(\underline{n}\times\underline{q}) = \epsilon_{ijk}\epsilon_{jlm}(n_l q_m)_k\,\underline{e}_i = -\epsilon_{jik}\epsilon_{jlm}(n_{l,k}q_m + n_l q_{m,k})$$
$$= -(\delta_{il}\delta_{km} - \delta_{im}\delta_{kl})(n_{l,k}q_m + n_l q_{m,k}) = -(n_{i,k}q_k - q_i n_{k,k} + n_i q_{k,k} - n_k q_{i,k})$$
$$\underline{n}\cdot\underline{\text{curl}}\,(\underline{n}\times\underline{q}) = -(q_k n_i n_{i,k} - q_i n_i n_{k,k} + q_{k,k} - q_{i,k}n_i n_k) = q_i n_i n_{k,k} - q_{k,k} + q_{i,k}n_i n_k$$
$$= q_i n_i n_{k,k} - D_{ti}q_i$$

since $n_i n_{i,k} = 0$ ($\|\underline{n}\| = 1$). Hence

$$\int_{\partial V} \underline{D}_t\cdot\underline{q}\, dS = \int_{\partial V} \underline{q}\cdot\underline{n}\,(\text{div}\,\underline{n})\, dS - \int_{\partial V} \underline{n}\cdot\underline{\text{curl}}\,(\underline{n}\times\underline{q})\,dS$$

$$\mathscr{I}^{(i)}(c^\star, \mathscr{D}) = - \int_{\mathscr{D}} \left((\underline{J} - \underset{\sim}{K} \cdot \nabla) \cdot \nabla \right) c^\star \, dV$$

$$+ \int_{\partial\mathscr{D}} \left((\underline{J} - \underset{\sim}{K} \cdot \nabla).\underline{n} + (\underline{n} \cdot \underset{\sim}{K} \cdot \underline{n}) 2\mathscr{C} - \underline{D}_t \cdot (\underset{\sim}{K} \cdot \underline{n}) \right) c^\star \, dS + \int_{\partial\mathscr{D}} \left(\underline{n} \cdot \underset{\sim}{K} \cdot \underline{n} \right) D_n c^\star \, dS \tag{16.97}$$

where $\mathscr{C}$ is the mean surface curvature. The form of the surface contribution can be deduced from the previous calculation:

$$\mathscr{I}^{(c)}(c^\star, \mathscr{D}) = \int_{\partial\mathscr{D}} (jc^\star + kD_n c^\star) \, dS \tag{16.98}$$

where j and k are generalized prescribed mass flux surface densities. External contributions take the form:

$$\mathscr{I}^{(e)}(c^\star, \mathscr{D}) = \int_{\mathscr{D}} (\gamma c^\star + \underline{\gamma} \cdot \nabla c^\star + \underset{\sim}{\gamma} : \nabla\nabla c^\star) \, dV = \int_V \left(\gamma - \underline{\gamma} \cdot \nabla + \underset{\sim}{\gamma} \cdot \nabla \cdot \nabla \right) c^\star \, dV$$

$$+ \int_{\partial V} \left(\underline{\gamma} \cdot \underline{n} - (\underset{\sim}{\gamma} \cdot \nabla) \cdot \underline{n} - \underline{D}_t \cdot (\underset{\sim}{\gamma} \cdot \underline{n}) + 2\mathscr{C}\underline{n} \cdot \underset{\sim}{\gamma} \cdot \underline{n} \right) c^\star \, dS + \int_{\partial V} \underset{\sim}{\gamma} : (\underline{n} \otimes \underline{n}) D_n c^\star \, dS \tag{16.99}$$

The last contribution $\mathscr{I}^{(a)}(c^\star, \mathscr{D})$ keeps the classical form (16.91).

The variational principle (16.89) is invoked again to derive the field equations:

$$\dot{c} = -\underline{J}^{eff} \cdot \nabla + \gamma \tag{16.100}$$

with the effective[3] tensor diffusion flux defined as

$$\underline{J}^{eff} = \underline{J} + \underline{\gamma} - (\underset{\sim}{K} + \underset{\sim}{\gamma}) \cdot \nabla \tag{16.101}$$

The associated boundary conditions for simple and double flux are

$$j = \underline{J}^{eff} \cdot \underline{n} + 2R(\underset{\sim}{K} + \underset{\sim}{\gamma}) : (\underline{n} \otimes \underline{n}) - ((\underset{\sim}{K} + \underset{\sim}{\gamma}) \cdot \underline{n}) \cdot \underline{D}_t,$$
$$k = (\underset{\sim}{K} + \underset{\sim}{\gamma}) : (\underline{n} \otimes \underline{n}) \tag{16.102}$$

The energy and entropy principles (isothermal case) take the following form

$$\dot{E} = \mathscr{I}^{(e)}, \quad \dot{\epsilon} = \gamma\dot{c} + \underline{\gamma} \cdot \nabla\dot{c} + \underset{\sim}{\gamma} : \nabla\nabla\dot{c}, \quad T\dot{S} \geq \int_{\partial V} T\underline{\Phi} \cdot \underline{n} \, dV \tag{16.103}$$

The last term vanishes due to Stokes theorem: $\int_S (\mathrm{curl}\ \underline{A}) \cdot \underline{n}\ dS = -\oint_\Gamma \underline{A} \cdot \underline{l}\ dl$ and $\Gamma = \emptyset$ for a closed surface. Finally, note that

$$n_{k,l} = D_{tl}n_k + n_{k,j}n_k n_l \Longrightarrow n_{k,k} = D_{tk}n_k, \quad \mathrm{div}\,\underline{n} = \underline{D}_t \cdot \underline{n} \qquad \square$$

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[3] This is similar to Germain's effective stress whose divergence arises in the strain gradient balance of momentum equation.

In contrast to the formulation (16.83), there is no internal energy contribution due to composition rate and its gradient (only the source terms $\gamma, \underline{\gamma}, \underset{\sim}{\gamma}$), as in the classical case. The new contributions are included in the extended entropy flux (Maugin and Muschik, 1994):

$$T\underline{\Phi} = \mu \underline{J}^{eff} + T\underline{\Phi}^{extra} \tag{16.104}$$

The Clausius–Duhem inequality (for vanishing $\gamma, \underline{\gamma}, \underset{\sim}{\gamma} \equiv 0$) then reads

$$-\dot{\psi} - \nabla \cdot (T\underline{\Phi}^{extra}) - \nabla \cdot (\mu \underline{J}^{eff}) \geq 0$$

$$-\left(\frac{\partial \psi}{\partial c} - \nabla \cdot \frac{\partial \psi}{\partial \nabla c} - \mu\right)\dot{c} - \nabla \cdot \left(T\underline{\Phi}^{extra} + \frac{\partial \psi}{\partial \nabla c}\dot{c}\right) - \underline{J}^{eff} \cdot \nabla \mu \geq 0$$

The chemical potential is now defined as

$$\mu = \frac{\partial \psi}{\partial c} - \nabla \cdot \frac{\partial \psi}{\partial \nabla c} \tag{16.105}$$

The following constitutive choices are made ensuring positivity of dissipation:

- extra–entropy flux

$$T\underline{\Phi}^{extra} = -\frac{\partial \psi}{\partial \nabla c}\dot{c} \tag{16.106}$$

- generalized Fick law

$$\underline{J}^{eff} = -\underset{\sim}{\kappa} \cdot \nabla \mu \tag{16.107}$$

- corresponding constitutive equations for $\underline{J}$ and $\underset{\sim}{K}$

$$\underline{J}^{eff} = \underline{J} - \underset{\sim}{K} \cdot \nabla = -\underset{\sim}{\kappa} \cdot (\nabla(\frac{\partial \psi}{\partial c} - \nabla \cdot \frac{\partial \psi}{\partial \nabla c})) \tag{16.108}$$

with

$$\underline{J} = -\underset{\sim}{\kappa} \cdot \frac{\partial \psi}{\partial c}, \quad \underset{\sim}{K} = -(\nabla \cdot \frac{\partial \psi}{\partial \nabla c})\underset{\sim}{\kappa} \tag{16.109}$$

(for uniform diffusion coefficients $\underset{\sim}{\kappa}$).

16.6 Conclusions

The development of continuum theories involving the gradient of field variables requires the introduction of suited (conjugate) generalized forces and stresses fulfilling higher order or additional balance equations. Such models can be constructed in an efficient and rigorous manner by applying the method of virtual power. It has been illustrated in the case of gradient and micromorphic plasticity and can be extended to damage and other internal variable theories in a straightforward way. The application to nonmechanical fields like temperature, microtemperature, concentration or microconcentration was shown to be possible even though it remains rather formal.

It provides new higher order diffusion equations that can be compared to existing ones derived from different concepts. For instance, micromechanically motivated higher-order continuum formulation of linear thermal conduction was proposed in Temizer and Wriggers (2010) based on a second gradient of temperature model very close to the formulation proposed in Sect. 16.5.3. In particular the higher order boundary conditions are the same. These boundary conditions, involving surface curvature effects, differ from the ones derived by means of an additional balance laws in Subsect. 16.5.2. Two different views of the Cahn–Hilliard model were presented, one based on an additional balance equation, the second one based on second gradient diffusion theory, all derived using the method of virtual power. The different inter-play between generalized forces and the use of extra–entropy flux leads to different boundary conditions. This combination of kinematic and constitutive choices was discussed many times by G.A. Maugin who tried in each situation to reduce the arbitrariness in the choice of generalized forces and extra–entropy flux vectors.

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