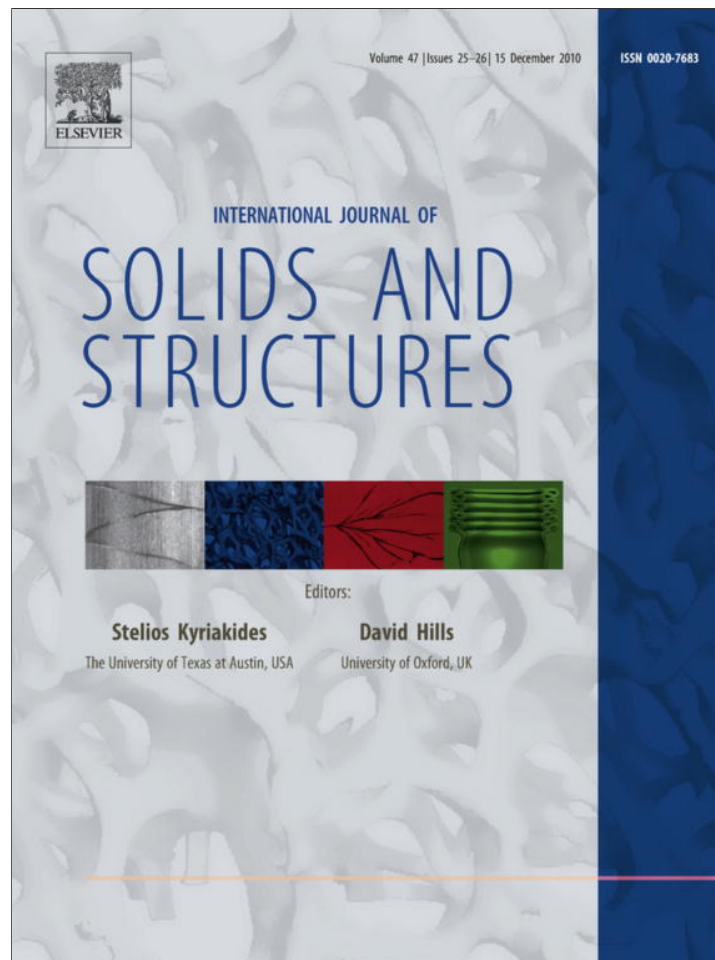


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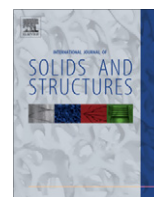
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## Some links between recent gradient thermo–elasto–plasticity theories and the thermomechanics of generalized continua

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## ABSTRACT

This work elaborates upon two robust models of gradient elasticity and gradient plasticity, and one gradient model of heat transfer, as originally advocated by the second author in the 1980's. The objective is, after recalling the links between these models and existing generalized continuum theories as developed in the 1960's and subsequently, to apply the same methodology to the case of diffusion with a view to establishing generalized transport equations. Aifantis double diffusivity and conductivity theory that provides generalized mass or heat transfer equations is compared to micromorphic-type hyper-temperature and micro-entropy proposals. The double temperature and the micromorphic thermal models are shown to lead to equations more general than Cattaneo's. The sign of the coefficient of the second time-derivative of temperature is found to differ according to both approaches. The double temperature model contains a fourth space derivative term not present in the micromorphic models. Such generalized equations can be useful, for example, in the interpretation of recent femtosecond laser experiments on metals.

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## 1. Introduction

While multiscale modeling procedures combining atomistic simulations (based on empirical potentials) with finite element calculations (based on standard elasticity or plasticity theory) are routinely used today for modeling mechanical behavior at micro and nano regimes, it seems that an extended continuum mechanics framework may still be useful for describing thermomechanical processes at submicron scales in an effective and computationally robust manner. In fact, continuum elasticity theory has been used successfully to model the response of nanotubes, in good agreement with respective molecular dynamics (MD) simulations, e.g. (Ru (2003)) and references quoted therein. More recently, generalized continuum elasticity theories of a nonlocal or gradient type have also been used to capture the mechanical behavior of nanotubes, e.g. (Zhang et al., 2005; Wang and Hu, 2005; Askes and Aifantis, 2009). Recent advances in gradient theory for elasticity, plasticity and dislocation dynamics have been reviewed by the second author (Aifantis, 2003). Gradient plasticity contributions, in particular, can be found in recent articles by various authors, e.g. (Fleck and Hutchinson, 2001), as well as the very recent article by Gurtin and Anand (2009), exclusively elaborating on continuum thermody-

amic aspects of the early models of Aifantis and Fleck & Hutchinson. Two schools of thought can be distinguished: one based on the kinetic nature of the carriers of plastic deformation and the other upon the concept of geometrically necessary dislocations.

Higher order or generalized theories of elastic continua, in particular, have been proposed in the 1900s (Cosserat) and later in 1960–70s (Mindlin, Toupin, Eringen, etc.), but these developments involved too many phenomenological coefficients (usually undetermined) and their applicability was examined mainly in relation to wave propagation studies. One may distinguish between “higher grade” theories, initiated by Mindlin, that introduce higher gradients of the displacement field in addition to the usual strain tensor, and “higher order” continuum media that introduce additional degrees of freedom, such as Cosserat continua and Eringen's micromorphic model (Eringen, 1999). As a result, we have, on the one hand, a well-established framework for higher grade and higher order theories and, on the other hand, independently developed simplified or specialized physically based models that turn out to be sufficient for describing experimentally observed size effects. The connection between both approaches usually remains loose, which often leads to a multiplication of essentially similar models, or a confusion of advantages and disadvantages of the various methods proposed. Several groups of available approaches can be reconciled based on Eringen's general micromorphic framework and its extension to viscoplasticity, as recognized in several recent papers (Kirchner and Steinmann, 2005; Forest, 2009; Hirschberger

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and Steinmann, 2009). In the present work, we will first show how Mindlin strain gradient theory can be specialized to recover Aifantis gradient elasticity model, together with the corresponding boundary conditions. A thermomechanical framework of Aifantis gradient plasticity theory has been provided by several authors (Forest et al., 2002; Gurtin and Anand, 2009; Fleck and Willis, 2009b) for models including the gradient of a scalar plastic measure, and (Forest and Sievert, 2003; Gurtin, 2003; Fleck and Willis, 2009a) for the gradient of the full plastic strain tensor. A different perspective was proposed by the first author (Forest, 2009) in the context of the micromorphic approach initiated by Eringen and Mindlin, as mentioned above. It will be shown in Section 2.2 that Aifantis gradient plasticity theory can be viewed as a micromorphic model with an internal constraint.

The higher order stresses in Mindlin's gradient theory are sometimes called hyperstresses. It may be anticipated that gradient theories can also be developed for transport phenomena and that there exist generalized forces to be referred in the sequel by analogy, as "hyper-temperature" or "hyper-entropy". Early works on generalized transport theory in media with microstructure (Aifantis, 1979, 1980b,a) already present the phenomenology of such enhanced heat or mass transport equations. The thermomechanics of generalized continua should again provide a suitable format for the formulation of coupled mechanics-based deformation theories with heat and diffusion effects. The case of generalized heat conduction is tackled in the present work, introducing generalized stresses in the spirit of the micromorphic approach. The corresponding phenomenology will be compared to Aifantis early derivations regarding heat propagation.

High temperature gradients are encountered in many thermo-mechanical processes, like thermal treatments of surfaces by means of nano or femtosecond lasers (Valette et al., 2005a). The validity of the classical heat equation can be questioned in such situations and generalized heat equations have been used to interpret these experiments. Most of them (e.g. the generalized thermoelastic model in Sharma (2008)) introduce the second time derivative of temperature following Cattaneo's initial proposal derived from statistical mechanics arguments (Cattaneo, 1958). Various methods exist for establishing enhanced heat equations applicable in the context of strong temperature gradient and fast transients. Extended thermodynamics has been designed for that purpose (Müller and Ruggeri, 1993). Generalized heat equations can also be obtained based on two-temperature models as initiated in Aifantis (1980a). For instance, one temperature variable is attributed to each phase in the homogenization of porous media, e.g. (Rees, 2010). In the homogenization procedure proposed in Cho et al. (2009) for granular media, there is one temperature for grains and one temperature for the matrix. In the context of laser applications, the two temperature model has been shown to be well adapted to the analysis of the thermal diffusion in metals irradiated by ultrashort laser pulses. It is based on the assumption that the electrons on the one hand and the ions on the other hand can be treated as two distinguishable subsystems, an electron gas and a phonon bath, represented by two temperatures. Finite element simulations of such models have been performed in Valette et al. (2005b) in order to estimate the size of the heat affected zone which can be compared to experimental observations. A mean temperature can be defined that satisfies a heat equation of higher order.

The objective of this paper is to show that the discussed generalized continuum mechanical theory can be extended to diffusion processes in order to obtain generalized transport equations. We explore how far the idea that energy can be stored or dissipated by means of strain gradient can be extended to the case of temperature or entropy gradients. It will be seen that additional terms, especially higher order partial derivatives, arise compared to

Cattaneo's equation. The results will also be compared to the prediction of double temperature models.

In particular, several new contributions are pointed out in this work: a fourth order spatial derivative of temperature in the double temperature model that exists when conductivities of both phases are comparable, a second time derivative of temperature further extending the hyperentropy theory from (Forest and Amestoy, 2008) and, finally, the formulation of a microentropy theory.

The plan of the article is as follows. Generalized continuum and strain gradient mechanics are reviewed in Section 2.1 in order to settle the framework subsequently applied to diffusion processes. The micromorphic approach is introduced in Section 2.2 in the mechanical context. A mixture type of approach, based on Aifantis double temperature model, is elaborated upon in Section 3.1 in order to derive a generalized form of the heat equation. On the other hand, the micromorphic approach, applied to temperature or entropy, also delivers higher order heat equations that are compared to Aifantis' one in Sections 3.2 and 3.3.

## 2. Gradient elasticity and plasticity

### 2.1. Link between second gradient theory and the gradient elasticity model

A most general form of a strain gradient theory has been established by Mindlin in the early 1960s. It assumes that not only the strain but also the strain gradient play a role in the material response. Its application to linear isotropic elasticity is presented in an exhaustive way in Mindlin and Eshel (1968). It is shown in particular that formulations based on the second gradient of the displacement or on the first gradient of the (symmetric) strain tensor are equivalent, since these variables are related by a compatibility relation. The balance equations and boundary conditions for the second gradient medium have also been derived by Germain (1973) based on the method of virtual power. According to Mindlin and Germain, the dual quantities of the first and second gradients of the displacement field in the work density of internal forces,  $w^{(i)}$ , are the second rank simple force stress tensor  $\sigma$  and the third rank double force stress tensor or hyperstress tensor  $\underline{S}$ :

$$w^{(i)} = \underline{\sigma} : \nabla \underline{u} + \underline{S} : \nabla \nabla \underline{u} = \sigma_{ij} u_{i,j} + S_{ijk} u_{i,jk} \quad (1)$$

These stress tensors display the following symmetry properties:

$$\sigma_{ij} = \sigma_{ji}, \quad S_{ijk} = S_{ikj} \quad (2)$$

In the static case and in the absence of volume (simple, double nor triple) forces, these stress tensors must fulfill the balance of momentum equation in the form:

$$\text{div } \underline{\tau} = 0, \quad \tau_{ijj} = 0 \quad (3)$$

where  $\underline{\tau}$  is the effective stress tensor defined by

$$\underline{\tau} = \underline{\sigma} - \text{div } \underline{S}, \quad \tau_{ij} = \sigma_{ij} - S_{ijk,k} \quad (4)$$

The boundary conditions associated with the partial differential Eq. (3) are quite intricate. They involve the normal and tangent gradient operators,  $D$  and  $\underline{D}$  respectively, of vector fields on a surface of normal  $\underline{n}$ :

$$\nabla \underline{u} = \underline{u} \otimes \underline{D} + \underline{D} \underline{u} \otimes \underline{n}, \quad \text{with } \underline{D} \underline{u} = \nabla \underline{u} \cdot \underline{n} \quad (5)$$

i.e.

$$D_j u_i = u_{i,j} - u_{i,k} n_k n_j \quad (6)$$

The simple traction vector  $\underline{t}$  and the double traction vector  $\underline{M}$  on a surface are related to the simple force, double force and hyperstress tensors in the following way:

$$\underline{\mathbf{t}} = \underline{\tau} : \underline{\mathbf{n}} + 2R\underline{\mathbf{S}} : (\underline{\mathbf{n}} \otimes \underline{\mathbf{n}}) - (\underline{\mathbf{S}} \cdot \underline{\mathbf{n}}) \cdot \underline{\mathbf{D}}, \quad \underline{\mathbf{M}} = \underline{\mathbf{S}} : (\underline{\mathbf{n}} \otimes \underline{\mathbf{n}}) \quad (7)$$

$$t_i = \tau_{ij}n_j + 2RS_{ijk}n_jn_k - D_j(S_{ijk}n_k), \quad M_i = S_{ijk}n_jn_k \quad (8)$$

where  $R = \underline{\mathbf{D}} \cdot \underline{\mathbf{n}} / 2 = D_i n_i / 2$  is the mean curvature radius of the surface at a given point.

The linear elasticity tensors relate the stress tensors to the strain and second gradient of displacement. In the case of a centro-symmetric system, there is no coupling between the constitutive equations which take the form:

$$\underline{\sigma} = \underline{\mathbf{C}} : \underline{\boldsymbol{\varepsilon}}, \quad \sigma_{ij} = C_{ijkl} \varepsilon_{kl} \quad (9)$$

$$\underline{\mathbf{S}} = \underline{\mathbf{A}} : \nabla \nabla \underline{\mathbf{u}}, \quad S_{ijk} = A_{ijklmn} u_{l,mn} \quad (10)$$

The expressions of the tensors of elastic moduli have been given in the isotropic case in Mindlin and Eshel (1968). They involve 5 independent moduli in addition to the two usual Lamé constants.

A special case of the previous theory has been considered by various authors (Shu, 1998; Shu and Fleck, 1999; Lazar et al., 2006) in order to reduce the complexity of the higher order constitutive equations. It amounts to formulating the constitutive equation for the higher order stress as if the hyperstress tensor  $\underline{\mathbf{S}}$  would coincide with the stress gradient  $\underline{\sigma} \otimes \nabla$ . Such a constraint may not be true in general since a strain gradient model differs from a stress gradient theory. It should thus be regarded as a simplifying constitutive assumption. An internal length  $l_c^2$  is introduced such that

$$\underline{\mathbf{S}} \equiv l_c^2 \underline{\sigma} \otimes \nabla, \quad S_{ijk} \equiv l_c^2 \sigma_{ij,k} \quad (11)$$

This assumption is sometimes related to Eringen's isotropic non local elasticity (Eringen, 2002). As a result of constitutive relation (9) and assuming homogeneous elasticity, we obtain

$$\underline{\mathbf{S}} = l_c^2 \underline{\sigma} \otimes \nabla = l_c^2 \underline{\mathbf{C}} : \underline{\boldsymbol{\varepsilon}} \otimes \nabla, \quad S_{ijk} = l_c^2 \sigma_{ij,k} = l_c^2 C_{ijmnl} \varepsilon_{mnl} \quad (12)$$

It is not clear how far the internal constraint between second and third rank stresses can actually be enforced in the second gradient theory. However, it can serve as a motivation to postulate the simplified higher order constitutive Eq. (12) which involves a single additional parameter, instead of the numerous parameters in the general isotropic relation (10). An analogous derivation has been given by the second author for nanostructured materials (Aifantis, 2009a).

In the case of isotropic linear elasticity, the second order stress  $\underline{\sigma}$  is related to the strain tensor by

$$\underline{\sigma} = \lambda(\text{tr } \underline{\boldsymbol{\varepsilon}}) \underline{\mathbf{1}} + 2\mu \underline{\boldsymbol{\varepsilon}} \quad (13)$$

The simplification (12) gives

$$\underline{\mathbf{S}} = l_c^2 (\lambda(\text{tr } \underline{\boldsymbol{\varepsilon}}) \underline{\mathbf{1}} + 2\mu \underline{\boldsymbol{\varepsilon}}) \otimes \nabla \quad (14)$$

When inserted into the definition of the effective stress tensor (4), the following constitutive equation between the second order effective stress and the strain tensor is obtained:

$$\underline{\tau} = \lambda(\text{tr } \underline{\boldsymbol{\varepsilon}}) \underline{\mathbf{1}} + 2\mu \underline{\boldsymbol{\varepsilon}} - c \nabla^2 (\lambda(\text{tr } \underline{\boldsymbol{\varepsilon}}) \underline{\mathbf{1}} + 2\mu \underline{\boldsymbol{\varepsilon}}) \quad (15)$$

This is exactly the expression of the gradient elasticity model with  $c = l_c^2$ , proposed and extensively used by Aifantis (1992), Altan and Aifantis (1997). In the absence of volume forces nor double/triple forces, the effective stress is divergence free, which makes the problem look like a standard first gradient model. However the boundary conditions still take the complicated form (7).

## 2.2. Link between Eringen's micromorphic model and Aifantis strain gradient plasticity

The micromorphic theory has been proposed simultaneously by Eringen and Mindlin (Mindlin, 1964; Eringen and Suhubi, 1964). It consists of introducing a general non compatible field of micro-deformation, in addition to the usual material deformation gradient, accounting for the deformation of a triad of microstructural directions. When the micro-deformation coincides with the deformation gradient, the micromorphic model reduces to the previous strain gradient theory. The micromorphic approach can, in fact, be applied to any macroscopic quantity in order to introduce an intrinsic length scale in the original standard continuum model in a systematic way, as done in Forest (2009). It is recalled here in relation to plastic strain and is shown to deliver, under special circumstances, the well-known Aifantis strain gradient plasticity model.

First the reference standard continuum plasticity model is presented before extending it to incorporate length scale effects. As usual, the total strain is split into its elastic and plastic parts:

$$\underline{\boldsymbol{\varepsilon}} = \underline{\boldsymbol{\varepsilon}}^e + \underline{\boldsymbol{\varepsilon}}^p \quad (16)$$

The reference state space corresponding to a classical elastoplasticity model is

$$DOFO = \{\underline{\mathbf{u}}\}, \quad STATEO = \{\underline{\boldsymbol{\varepsilon}}^e, p, \alpha\} \quad (17)$$

where  $\underline{\boldsymbol{\varepsilon}}^e$  is the (infinitesimal) elastic strain tensor,  $p$  the cumulative plastic strain variable and  $\alpha$  denotes another possible internal variable of any tensorial rank, see, for example, (Mauguin and Muschik, 1994). The original set of degrees of freedom *DOFO* contains the displacement vector of each material point  $\underline{\mathbf{u}}(\underline{\mathbf{x}})$ . A standard yield function and a corresponding dissipation potential can be used to compute plastic flow and the evolution equations for the other internal variables.

According to the micromorphic approach, a microstrain variable  $\varepsilon_p$  is associated to  $p$  and regarded as an additional degree of freedom. The material behavior is then assumed to depend on the micromorphic variable and its gradient. Accordingly, the sets of degrees of freedom and the state space are enhanced as follows:

$$DOF = \{\underline{\mathbf{u}}, \varepsilon_p\}, \quad STATE = \{\underline{\boldsymbol{\varepsilon}}^e, p, \alpha, \varepsilon_p, \nabla \varepsilon_p\} \quad (18)$$

The principle of virtual power is generalized to incorporate the microstructural effects. This represents a systematic use of the method of virtual power that Germain applied to Eringen's micromorphic medium (Germain, 1973). The classical powers of internal and contact forces are extended in the following way:

$$p^{(i)} = \underline{\sigma} : \underline{\dot{\boldsymbol{\varepsilon}}} + a \dot{\varepsilon}_p + \underline{\mathbf{b}} \cdot \nabla \dot{\varepsilon}_p, \quad p^{(e)} = \underline{\mathbf{t}} \cdot \underline{\dot{\mathbf{u}}} + a^e \dot{\varepsilon}_p \quad (19)$$

in which generalized stresses  $a$  and  $\underline{\mathbf{b}}$  have been introduced. The application of the method of virtual power leads to the following additional local balance equation and boundary conditions, in addition to the classical local balance of momentum and traction conditions at the outer boundary:

$$\text{div } \underline{\mathbf{b}} - a = 0, \quad \forall \underline{\mathbf{x}} \in \Omega, \quad a^e = \underline{\mathbf{b}} \cdot \underline{\mathbf{n}}, \quad \forall \underline{\mathbf{x}} \in \partial\Omega \quad (20)$$

Generalized body forces could be introduced in case of necessity in the balance equations. The microstructural effects therefore arise in the balance of energy in the form:

$$\rho \dot{\epsilon} = p^{(i)} - \text{div } \underline{\mathbf{q}} + \rho r \quad (21)$$

where  $\epsilon$  is the specific internal energy,  $\underline{\mathbf{q}}$  the heat flux vector and  $r$  denotes external heat sources. The free energy density function  $\psi$  is

assumed to be a function of the previous set *STATE*. The entropy principle is formulated in the form of the Clausius–Duhem inequality

$$-\rho(\dot{\psi} + \eta\dot{T}) + p^{(i)} - \frac{\mathbf{q}}{T} \cdot \nabla T \geq 0 \quad (22)$$

where  $\eta$  is the entropy density function and where the thermal contribution is included. In this work, the following state laws are postulated:

$$\underline{\underline{\sigma}} = \rho \frac{\partial \psi}{\partial \underline{\underline{\mathbf{e}}^e}, \quad a = \rho \frac{\partial \psi}{\partial \lambda p}, \quad \underline{\underline{\mathbf{b}}} = \rho \frac{\partial \psi}{\partial \nabla \lambda p}, \quad R = \rho \frac{\partial \psi}{\partial p}, \quad X = \rho \frac{\partial \psi}{\partial \alpha} \quad (23)$$

State equations relate the generalized stresses to the microstrain variable and its gradient, assuming, for simplicity, that no dissipation is associated with them. This restriction will be sufficient to recover the targeted class of models. The thermodynamical forces associated with internal variables are  $R$  and  $X$ . The residual dissipation therefore is

$$D^{res} = \underline{\underline{\sigma}} : \dot{\underline{\underline{\mathbf{e}}}}^p - R\dot{p} - X\dot{\alpha} \geq 0 \quad (24)$$

as in the classical case. The plastic behavior is characterized by the yield function  $f(\underline{\underline{\sigma}}, R, X)$ . In the micromorphic model, the yield function can still be treated as the dissipation potential providing the flow and evolution rules for internal variables. This corresponds to the hypothesis of maximal dissipation:

$$\dot{\underline{\underline{\mathbf{e}}}}^p = \dot{\lambda} \frac{\partial f}{\partial \underline{\underline{\sigma}}}, \quad \dot{p} = -\dot{\lambda} \frac{\partial f}{\partial R}, \quad \dot{\alpha} = -\dot{\lambda} \frac{\partial f}{\partial X} \quad (25)$$

where  $\dot{\lambda}$  is the plastic multiplier. At this stage, a coupling between the macroscopic and microscopic variables must be introduced, for instance via the relative cumulative plastic strain  $p - \lambda p$ .

A quadratic form is now proposed for the free energy density function, with respect to elastic strain, cumulative plastic strain, relative plastic strain and micromorphic plastic strain gradient:

$$\rho\psi(\underline{\underline{\mathbf{e}}}^e, p, \lambda p, \nabla \lambda p) = \frac{1}{2} \underline{\underline{\mathbf{e}}}^e : \underline{\underline{\mathbf{C}}} : \underline{\underline{\mathbf{e}}}^e + \frac{1}{2} H p^2 + \frac{1}{2} H_\chi (p - \lambda p)^2 + \frac{1}{2} A \nabla \lambda p \cdot \nabla \lambda p \quad (26)$$

The corresponding classical model describes an elastoplastic material behavior with linear elasticity characterized by the tensor of elastic moduli  $\underline{\underline{\mathbf{C}}}$  and the linear hardening modulus  $H$ . Isotropy has been assumed for the last term for the sake of brevity. Two additional material parameters are introduced in the micromorphic extension of this classical model, namely the coupling modulus  $H_\chi$  (unit MPa) and the micromorphic stiffness  $A$  (unit MPa.mm<sup>2</sup>). The thermodynamic forces associated with the state variables are given by the relations (23):

$$\underline{\underline{\sigma}} = \underline{\underline{\mathbf{C}}} : \underline{\underline{\mathbf{e}}}^e, \quad a = -H_\chi (p - \lambda p), \quad \underline{\underline{\mathbf{b}}} = A \nabla \lambda p, \quad R = (H + H_\chi)p - H_\chi \lambda p \quad (27)$$

Note that when the relative plastic strain  $e = p - \lambda p$  is close to zero, the linear hardening rule retrieves its classical form and the generalized stress  $a$  vanishes. Only the strain gradient effect  $\nabla p$  remains in the enriched work of internal forces (19). This is the situation encountered in the strain gradient plasticity models developed in Fleck and Hutchinson (2001). When inserted in the additional balance Eq. (20), the previous state laws lead to the following partial differential equation:

$$\lambda p - \frac{A}{H_\chi} \Delta \lambda p = p \quad (28)$$

which is identical to the additional partial differential equation used in the so-called implicit gradient-enhanced elastoplasticity in Engelen et al. (2003). The microstrain  $\lambda p$  is called there the “non local strain measure”  $\bar{p}$ . Note however that the latter model involves only one additional material parameter, namely  $l_c^2 = A/H_\chi$  instead of two in the micromorphic approach. In the micromorphic approach, the coupling modulus  $H_\chi$  plays a central role and makes it possible to have a fully consistent thermomechanical basis for the model. When its value is high enough, it acts as a penalty term forcing the micromorphic plastic strain to follow the macroscopic one as close as possible.

The necessity of an additional boundary condition associated with the nonlocal strain measure has already been recognized in Engelen et al. (2003). The associated Neumann condition is used in the form:

$$\nabla \lambda p \cdot \underline{\underline{\mathbf{n}}} = 0 \quad \text{on} \quad \partial \Omega \quad (29)$$

It coincides with the more general boundary condition derived in the micromorphic approach:

$$\underline{\underline{\mathbf{b}}} \cdot \underline{\underline{\mathbf{n}}} = a^c \quad \text{on} \quad \partial \Omega \quad (30)$$

when  $a^c = 0$  and when  $\underline{\underline{\mathbf{b}}}$  is linear with respect to  $\nabla \lambda p$ , as it is the case for the quadratic potential (26).

The yield function is now chosen as

$$f(\underline{\underline{\sigma}}, R) = \sigma_{eq} - \sigma_Y - R \quad (31)$$

where  $\sigma_{eq}$  is an equivalent stress measure and  $\sigma_Y$  the initial yield stress. The hardening rule then takes the following form:

$$R = \rho \frac{\partial \psi}{\partial p} = (H + H_\chi)p - H_\chi \lambda p \quad (32)$$

After substituting the balance Eq. (28) into the hardening law, yielding takes place when

$$\sigma_{eq} = \sigma_Y + H \lambda p - A \left( 1 + \frac{H}{H_\chi} \right) \Delta \lambda p \quad (33)$$

This expression coincides with the enhanced yield criterion originally proposed for gradient plasticity (Aifantis, 1984, 1987; Forest et al., 2002) and used for strain localization simulations in de Borst et al. (1993), de Borst and Pamin (1996), de Borst et al. (1999) when the micromorphic variable remains as close as possible to the plastic strain:  $\lambda p \simeq p$ . In the original work, the Laplace operator is directly introduced in the yield function either as a postulate, or as a consequence of dislocation flux in the elementary volume, whereas its presence is derived here from the combination of the additional balance equation and the linear generalized constitutive equations.

As a result, Aifantis' model has been retrieved from the micromorphic approach by choosing simple linear constitutive equations and introducing the internal constraint  $\lambda p \equiv p$  stating that the micromorphic variable coincides with the plastic strain itself. The original Aifantis model can also be directly constructed through a gradient type of internal variable model, as already done by several authors (Forest et al., 2002; Forest and Sievert, 2003; Gurtin, 2003). In particular, a recent contribution (Gurtin and Anand, 2009) rests upon the energy storage due to gradient of plastic strain to derive this class of models in the same way as Forest et al. (2002). More general dissipative mechanisms can also be added.

### 3. Gradient theories of thermal conduction in solids

Higher order gradient effects also play an important role in the diffusion of atoms and heat in solids, especially in nano and microdevices (Gad-el-Hak, 2004) or in the presence of strong gradients as in thermal chocks (Dreyer and Struchtrup, 1993; Bargmann and Steinmann, 2008). Generalized diffusion equations have been phenomenologically derived in Cahn and Hilliard (1958), by including interfacial energy, and in Aifantis (1980b) based on mixture theory. The enhancement of the classical partial differential equation consists of higher order spatial gradients of concentration, on the one hand, and of higher order time derivatives, on the other hand, so as to obtain a hyperbolic diffusion equation. Similar extensions hold for the heat equation, as advocated by Cattaneo (1958) who introduced the heat flux rate, and, later on, by Aifantis (1980a) based on a double temperature mixture type theory. Recently, the micromorphic approach, as sketched in Section 2.2, has been applied to the temperature variable itself, and two types of generalized heat equations were derived (Forest and Amestoy, 2008), using a method similar to one proposed by Fried and Gurtin (1993), Gurtin (1996), Maugin (2006) for mass diffusion and phase field theories. An extension of this gradient of entropy model is proposed in the following. The objective of this section is then to compare the results obtained by the double temperature and micromorphic theories. In particular, the derived partial differential equations will be discussed in each case. The discussion is limited to heat equations, as specific difficulties related to entropy must be tackled. However, similar analyses may easily be carried out for mass transport.

Section 3.1 summarizes Aifantis double temperature model, whereas Sections 3.2 and 3.3 envisage rigid heat conducting solids with single temperature but gradient of temperature or gradient of entropy effects.

#### 3.1. Double temperature and higher order gradients in the heat equation

According to mixture theory, see (Müller, 2001), the evolution of a multi-component system is governed by as many sets of balance equations as the constituents. The balance equations for mass, energy and momentum are coupled by source terms for which constitutive relationships must be proposed. In the case of a heat conducting two-component system, partial mass densities<sup>1</sup>  $\rho_i$ , internal energies,  $\epsilon_i$ , heat fluxes,  $\mathbf{q}_i$  and temperatures,  $\theta_i$ , are introduced, that fulfill the following two energy balance equations:

$$\rho_1 \dot{\epsilon}_1 = -\text{div} \mathbf{q}_1 + \hat{\epsilon}_1, \quad \rho_2 \dot{\epsilon}_2 = -\text{div} \mathbf{q}_2 + \hat{\epsilon}_2 \quad (34)$$

where  $\hat{\epsilon}_i$  are source terms. In a mixture for which the partial densities are such that  $\rho_1 = \rho_2 = \rho/2$ , the macroscopic internal energy, and heat flux may be defined as

$$2\epsilon = \epsilon_1 + \epsilon_2, \quad 2\mathbf{q} = \mathbf{q}_1 + \mathbf{q}_2, \quad 2\theta = \theta_1 + \theta_2 \quad (35)$$

The expression for the macroscopic internal energy follows from its definition,  $\rho\epsilon = \rho_1\epsilon_1 + \rho_2\epsilon_2$ , and the specific hypothesis on densities, whereas the definition of temperature  $\theta$  is an assumption which is made in order to generate overall evolution partial differential equations. Alternative definitions exist, see for instance (Gouin and Ruggeri, 2008) where, however, the overall heat equation is not derived. In the absence of chemical reactions, the source terms are assumed to compensate

$$\hat{\epsilon}_1 + \hat{\epsilon}_2 = 0 \quad (36)$$

<sup>1</sup> The partial mass density  $\rho_1$  of a component 1 with mass  $\delta m_1$  inside a total volume  $\delta V$  is  $\rho_1 = \delta m_1 / \delta V$ . It follows that the total mass density of the material point is  $\rho = \rho_1 + \rho_2$ .

so that the global balance of energy reads:

$$\rho \dot{\epsilon} = -\text{div} \mathbf{q} \quad (37)$$

The entropy production due to each constituent is assumed to take the form

$$\rho \dot{\eta}_1 + \text{div} \frac{\mathbf{q}_1}{\theta_1} = \pi_1, \quad \rho \dot{\eta}_2 + \text{div} \frac{\mathbf{q}_2}{\theta_2} = \pi_2 \quad (38)$$

We require the total entropy production rate to be positive for all processes:

$$2\pi = \pi_1 + \pi_2 \geq 0 \quad (39)$$

Combining the partial balance of energy Eq. (34) and the entropy inequality (39), the following reduced Clausius–Duhem inequality is derived

$$\rho \left( 1 - \frac{1}{\theta_1} \frac{\partial \epsilon_1}{\partial \eta_1} \right) \dot{\eta}_1 + \rho \left( 1 - \frac{1}{\theta_2} \frac{\partial \epsilon_2}{\partial \eta_2} \right) \dot{\eta}_2 + \rho \left( \frac{\hat{\epsilon}_1}{\theta_1} + \frac{\hat{\epsilon}_2}{\theta_2} \right) - \frac{\mathbf{q}_1}{\theta_1} \cdot \frac{\nabla \theta_1}{\theta_1} - \frac{\mathbf{q}_2}{\theta_2} \cdot \frac{\nabla \theta_2}{\theta_2} \geq 0 \quad (40)$$

The state equations linking partial temperatures and entropies are then

$$\theta_1 = \frac{\partial \epsilon_1}{\partial \eta_1}, \quad \theta_2 = \frac{\partial \epsilon_2}{\partial \eta_2} \quad (41)$$

so that the residual dissipation rate is

$$\rho \left( \frac{\hat{\epsilon}_1}{\theta_1} + \frac{\hat{\epsilon}_2}{\theta_2} \right) - \frac{\mathbf{q}_1}{\theta_1} \cdot \frac{\nabla \theta_1}{\theta_1} - \frac{\mathbf{q}_2}{\theta_2} \cdot \frac{\nabla \theta_2}{\theta_2} \geq 0 \quad (42)$$

From now on, we adopt a linear setting, in the sense that temperature variations remain sufficiently small. The following analysis extends the one initiated by the second author (Aifantis, 1980a). A parallel can be drawn with the two-component diffusion or double diffusivity theory (Aifantis, 1979). The generalized Fourier laws, in the isotropic case, are assumed to take the form

$$\mathbf{q}_1 = -\kappa_{11} \nabla \theta_1 - \kappa_{12} \nabla \theta_2, \quad \mathbf{q}_2 = -\kappa_{21} \nabla \theta_1 - \kappa_{22} \nabla \theta_2 \quad (43)$$

Generalized specific heat capacities are also introduced in the form

$$\rho_1 \epsilon_1 = C_{11} \theta_1 + C_{12} \theta_2, \quad \rho_2 \epsilon_2 = C_{21} \theta_1 + C_{22} \theta_2 \quad (44)$$

where the  $C_{ij}$  are the generalized heat capacity coefficients. Within the assumed linear framework, the coupling term may be taken to be proportional to the temperature gap,  $\theta_1 - \theta_2$ :

$$\hat{\epsilon}_1 = -\hat{\epsilon}_2 = h(\theta_2 - \theta_1) \quad (45)$$

where  $h$  is a coupling (microscopic heat transfer) parameter. Within the linearized context,  $\theta_1$  and  $\theta_2$  remain close so that the residual dissipation rate (42) reduces to

$$-\frac{\mathbf{q}_1}{\theta_1} \cdot \frac{\nabla \theta_1}{\theta_1} - \frac{\mathbf{q}_2}{\theta_2} \cdot \frac{\nabla \theta_2}{\theta_2} \geq 0 \quad (46)$$

which is identically fulfilled when the symmetric part of the matrix  $\kappa_{ij}$  is positive definite. The sign of the coupling parameter  $h$  remains unspecified since the source terms cancel out in the inequality, within the linear approximation.

Upon substituting the above stated constitutive equations into the corresponding balance equations and assuming homogeneity of the body, the following system of partial differential equations is found:

$$C_{11} \dot{\theta}_1 + C_{12} \dot{\theta}_2 = \kappa_{11} \nabla^2 \theta_1 + \kappa_{12} \nabla^2 \theta_2 + h(\theta_2 - \theta_1) \quad (47)$$

$$C_{21} \dot{\theta}_1 + C_{22} \dot{\theta}_2 = \kappa_{21} \nabla^2 \theta_1 + \kappa_{22} \nabla^2 \theta_2 - h(\theta_2 - \theta_1) \quad (48)$$

that can be put into the following matrix form

$$\begin{bmatrix} C_{11} \frac{d}{dt} - \kappa_{11} \nabla^2 + h & C_{12} \frac{d}{dt} - \kappa_{12} \nabla^2 - h \\ C_{21} \frac{d}{dt} - \kappa_{21} \nabla^2 - h & C_{22} \frac{d}{dt} - \kappa_{22} \nabla^2 + h \end{bmatrix} \begin{bmatrix} \theta_1 \\ \theta_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \quad (49)$$

Elimination of  $\theta_1$  and  $\theta_2$  leads to the following higher order partial differential equation that must be fulfilled by the global temperature:

$$\begin{aligned} \dot{\theta} + \frac{C_{11}C_{22} - C_{12}C_{21}}{h(C_{11} + C_{22} + C_{12} + C_{21})} \ddot{\theta} &= \frac{\kappa_{11} + \kappa_{22} + \kappa_{12} + \kappa_{21}}{C_{11} + C_{22} + C_{12} + C_{21}} \nabla^2 \theta \\ &+ \frac{\kappa_{11}C_{22} + \kappa_{22}C_{11} + \kappa_{12}C_{21} + \kappa_{21}C_{12}}{h(C_{11} + C_{22} + C_{12} + C_{21})} \nabla^2 \dot{\theta} \\ &- \frac{\kappa_{11}\kappa_{22} - \kappa_{12}\kappa_{21}}{h(C_{11} + C_{22} + C_{12} + C_{21})} \nabla^4 \theta \end{aligned} \quad (50)$$

The first time derivative and the Laplacian of temperature are present in the classical heat equation. Additional terms comprise the second time derivative, the Laplacian of the temperature rate and the fourth order gradient of temperature. We recover the equation found by the second author (Aifantis, 1979) for mass diffusion after neglecting the coupling terms  $\kappa_{12} = \kappa_{21} = 0$ ,  $C_{12} = C_{21} = 0$ :

$$\begin{aligned} \dot{\theta} + \frac{C_{11}C_{22}}{h(C_{11} + C_{22})} \ddot{\theta} &= \frac{\kappa_{11} + \kappa_{22}}{C_{11} + C_{22}} \nabla^2 \theta + \frac{\kappa_{11}C_{22} + \kappa_{22}C_{11}}{h(C_{11} + C_{22})} \nabla^2 \dot{\theta} \\ &- \frac{\kappa_{11}\kappa_{22}}{h(C_{11} + C_{22})} \nabla^4 \theta \end{aligned} \quad (51)$$

Positivity of dissipation is ensured for  $\kappa_{11} > 0$  and  $\kappa_{22} > 0$ . The existence of a convex internal energy potential implies  $C_{11} > 0$  and  $C_{22} > 0$ . As a result, the coefficient in front of  $\nabla^2 \theta$  is positive, as it should be. A hyperbolic heat equation was proposed by Cattaneo (1958), based on kinetic theory arguments. The contributions of  $\dot{\theta}$  and  $\ddot{\theta}$  in the Eq. (51) can be compared directly to Cattaneo's equation when the signs of the coefficients in front of  $\dot{\theta}$  and  $\ddot{\theta}$  are positive. This happens for  $h > 0$ . Note that Cattaneo proposed an earlier version of the extended heat equation containing the  $\nabla^2 \dot{\theta}$  term, see (Müller and Ruggeri, 1993). For  $h > 0$ , the coefficients in front of  $\nabla^2 \dot{\theta}$  and  $\nabla^4 \theta$  are respectively positive and negative. The term  $\nabla^4 \theta$  seems to be new. It drops when one diffusion mechanism is more effective than the other one ( $\kappa_2 \ll \kappa_1$ ):

$$\dot{\theta} + \frac{C_{11}C_{22}}{h(C_{11} + C_{22})} \ddot{\theta} = \frac{\kappa_{11}}{C_{11} + C_{22}} \nabla^2 \theta + \frac{\kappa_{11}C_{22}}{h(C_{11} + C_{22})} \nabla^2 \dot{\theta} \quad (52)$$

If the second time derivative is dropped, we are left with

$$\dot{\theta} = \frac{\kappa_{11}}{C_{11} + C_{22}} \nabla^2 \theta + \frac{\kappa_{11}C_{22}}{h(C_{11} + C_{22})} \nabla^2 \dot{\theta} \quad (53)$$

which has the form of Cattaneo's first generalization of the heat equation. A double temperature model for a deformable porous elastic medium was proposed by the second author in 1980 (Aifantis, 1980a) and a higher gradient heat conduction equation for a plastically deforming medium (containing  $\nabla^2 \theta$  and  $\nabla^4 \theta$  terms) was also suggested by him in 1992 (Aifantis, 1992). This is also similar to Barenblatt's infiltration theory for the pore pressure in double porosity media as discussed earlier by the second author (Aifantis, 1980a).

### 3.2. Hyper-temperature or hyper-entropy in thermoelastic solids

The question of the storage of energy through the gradient of temperature or entropy is raised for rigid heat conducting solids, by analogy to the question of energy storage based on strain gradients discussed in Section 2.1. The proposed methodology is based on the micromorphic approach of Section 2.2 and closely related to the microforce formulation by Fried and Gurtin (1993), Gurtin (1996) developed for phase field and Cahn–Hilliard equations. We distinguish between the gradient of temperature theory and the gradient of entropy model (Forest and Amestoy, 2008).

#### 3.2.1. Gradient of temperature theory

As discussed recently in Forest (2009), the micromorphic approach can be applied to any element of the state space of a thermomechanical model. It can, in particular, be applied to the temperature variable  $\theta$  itself. Accordingly, we assume that there exist additional powers of internal generalized forces  $p^{(i)}$  and of contact generalized forces  $p^{(c)}$  in the form

$$p^{(i)} = a\dot{\theta} + \underline{b} \cdot \nabla \dot{\theta}, \quad p^{(c)} = a^c \dot{\theta} \quad (54)$$

where  $a$  and  $\underline{b}$  are generalized stresses, or so-called microforces according to Gurtin's terminology (Gurtin, 1996). These stresses contribute to the balance of energy

$$\rho \dot{\epsilon} = a\dot{\theta} + \underline{b} \cdot \nabla \dot{\theta} - \text{div} \underline{q} \quad (55)$$

For the sake of conciseness, the purely mechanical part of the problem is omitted. In the spirit of the micromorphic approach, a virtual power principle is assumed to hold for the generalized stresses  $a$  and  $\underline{b}$  so that they fulfill the following balance equation:

$$\text{div} \underline{b} - a = 0, \quad \forall \underline{x} \in V, \quad \underline{b} \cdot \underline{n} = a^c, \quad \forall \underline{x} \in \partial V \quad (56)$$

which shall hold in addition to the balance of energy. We consider rigid heat conducting solids endowed with a free energy density function that depends on temperature and temperature gradient,  $\psi(\theta, \nabla \theta) = \epsilon - \theta \eta$ . The Clausius–Duhem inequality takes the form

$$-\rho \eta \dot{\theta} - \rho \dot{\psi} + p^{(i)} - \underline{q} \cdot \frac{\nabla \theta}{\theta} \geq 0 \quad (57)$$

When expanded, it becomes

$$\left( a - \rho \eta - \rho \frac{\partial \psi}{\partial \theta} \right) \dot{\theta} + \left( \underline{b} - \rho \frac{\partial \psi}{\partial \nabla \theta} \right) \cdot \nabla \dot{\theta} - \underline{q} \cdot \frac{\nabla \theta}{\theta} \geq 0 \quad (58)$$

We first assume that the two first terms are non-dissipative and provide the state equations

$$\eta = -\frac{\partial \psi}{\partial \theta} + \frac{a}{\rho}, \quad \underline{b} = \rho \frac{\partial \psi}{\partial \nabla \theta} \quad (59)$$

The positivity of residual dissipation is then ensured by the choice of a classical Fourier law of the form:

$$\underline{q} = -\underline{\kappa} \cdot \nabla \theta \quad (60)$$

If the theory is linearized around temperature  $\theta_0$ , the free energy function is a quadratic potential in  $\theta$  and  $\nabla \theta$ :

$$\rho \psi(\theta, \nabla \theta) = -\frac{1}{2} \frac{\rho C}{\theta_0} (\theta - \theta_0)^2 + \frac{1}{2} A \nabla \theta \cdot \nabla \theta \quad (61)$$

where  $C$  is the specific heat coefficient and  $A$  is an additional material parameter for an isotropic heat-conducting solid. The heat equation is obtained from

$$\rho \theta \dot{\eta} = -\text{div} \underline{q} \quad (62)$$

which gives

$$\rho C_\epsilon \dot{\theta} = \kappa \nabla^2 \theta - \theta_0 A \nabla^2 \dot{\theta} \quad (63)$$

which has the same form as Cattaneo's first Eq. (53), as derived in the previous double temperature model. Concavity of the potential  $\psi$  in Eq. (61) would require  $A < 0$  which corresponds to  $h > 0$  in Eq. (53). Then both equations are indeed equivalent.

If the first term in (58) is dissipative, there exists a viscous generalized stress  $a^v$ ,

$$a^v = a - \rho \eta - \rho \frac{\partial \psi}{\partial \theta} \quad (64)$$

so that the residual dissipation is

$$a^v \dot{\theta} - \underline{q} \cdot \frac{\nabla \theta}{\theta} \geq 0 \quad (65)$$

A quadratic dissipation potential  $\Omega(a^v, \nabla\theta)$  is adopted:

$$\Omega(a^v, \nabla T) = \frac{1}{2\alpha} a^{v2} - \frac{1}{2} \nabla\theta \cdot \underline{\kappa} \cdot \nabla\theta \quad (66)$$

where  $\alpha$  is a material parameter. It follows that

$$\dot{\theta} = \frac{\partial\Omega}{\partial a^v} = \frac{1}{\alpha} a^v, \quad \underline{\mathbf{q}} = \frac{\partial\Omega}{\partial \nabla\theta} = -\underline{\kappa} \cdot \nabla\theta \quad (67)$$

In this context, assuming homogeneity and isotropy of the body, the heat Eq. (62) becomes, in the presence of a viscous generalized stress  $a^v$ :

$$\rho\theta\dot{\eta} - a^v \dot{\theta} = -\text{div} \underline{\mathbf{q}} \quad (68)$$

Taking the constitutive Eq. (67) into account, the contribution  $a^v \dot{\theta}$  is nonlinear in  $\dot{\theta}$  so that it can be neglected in order to finally obtain the following linearized generalized heat equation:

$$\rho C \dot{\theta} - \theta_0 \alpha \ddot{\theta} = \kappa \nabla^2 \theta - \theta_0 A \nabla^2 \dot{\theta} \quad (69)$$

The additional dissipative contribution therefore provides a second time derivative in the heat equation, in a similar way as in (52). However, the sign of the coefficient in front of  $\ddot{\theta}$  differs, since  $\alpha$  is necessarily positive here to ensure positivity of the first dissipation term in Eq. (65). In contrast, as already mentioned,  $A < 0$  leads to the same sign in the term in front of  $\nabla^2 \dot{\theta}$  in Eqs. (69) and (52) for  $h > 0$ .

Note that the additional balance Eq. (56) could be enhanced by introducing an “inertial” term  $\ddot{\theta}$ . Such a contribution leads to the presence of the third time derivative of temperature  $\dot{\theta}$  in the heat equation.

### 3.2.2. Gradient of entropy theory

In the mass diffusion equation, the gradient of chemical potential induces a mass flux that, in turn, leads to an evolution of concentration  $\dot{c}$ . The generalized mass diffusion theory in Gurtin (1996) introduces a linear power functional in  $\dot{c}$ . The Cahn–Hilliard diffusion equation is obtained in this way. Similarly, in the heat equation, the gradient of temperature,  $\nabla\theta$ , induces a heat flux,  $\underline{\mathbf{q}}$ , that, in turn, leads to an evolution equation for the entropy,  $\dot{\eta}$ . Accordingly, an extended heat conduction theory should proceed by introducing a linear power functional in entropy rate  $\dot{\eta}$ :

$$p^{(i)} = a\dot{\eta} + \underline{\mathbf{b}} \cdot \nabla\dot{\eta}, \quad p^{(c)} = a^c \dot{\eta} \quad (70)$$

The generalized stress tensors  $a$  and  $\underline{\mathbf{b}}$  are still assumed to fulfill the principle of virtual power that leads to the additional balance Eq. (56), with the associated boundary conditions. The additional power enters the energy equation:

$$\rho \dot{e} = a\dot{\eta} + \underline{\mathbf{b}} \cdot \nabla\dot{\eta} - \text{div} \underline{\mathbf{q}} \quad (71)$$

The Clausius–Duhem inequality is written in the form that includes the internal energy function:

$$\rho\theta\dot{\eta} - \rho\dot{e} + p^{(i)} - \underline{\mathbf{q}} \cdot \frac{\nabla\theta}{\theta} \geq 0 \quad (72)$$

Assuming the functional dependence  $\epsilon(\eta, \nabla\eta)$ , we obtain

$$\left( a + \rho\theta - \rho \frac{\partial\epsilon}{\partial\eta} \right) \dot{\eta} + \left( \underline{\mathbf{b}} - \rho \frac{\partial\epsilon}{\partial \nabla\eta} \right) \cdot \nabla\dot{\eta} - \underline{\mathbf{q}} \cdot \frac{\nabla\theta}{\theta} \geq 0 \quad (73)$$

Such a dependence of the internal energy on the gradient of entropy has already been considered to construct extended Cahn–Hilliard fluids (Casal and Gouin, 1988; Gouin and Ruggeri, 2005). The following state law is assumed to hold

$$\underline{\mathbf{b}} = \rho \frac{\partial\epsilon}{\partial \nabla\eta} \quad (74)$$

A viscous generalized stress  $a^v$  is introduced, so that the residual dissipation is:

$$a^v \dot{\eta} - \underline{\mathbf{q}} \cdot \frac{\nabla\theta}{\theta} \geq 0 \quad (75)$$

with

$$a^v = a + \rho\theta - \rho \frac{\partial\epsilon}{\partial\eta} \quad (76)$$

The choice of a dissipation potential of the form (66) leads to the relation

$$\theta = \frac{\partial\epsilon}{\partial\eta} + \frac{\alpha}{\rho} \dot{\eta} - \frac{a}{\rho} \quad (77)$$

If the theory is linearized around temperature  $\theta_0$ , the free energy function is a quadratic potential in  $\eta$  and  $\nabla\eta$ :

$$\rho\epsilon(\eta, \nabla\eta) = \rho\eta\theta_0 + \frac{\rho^2(\eta - \eta_0)^2}{4\beta} + \frac{1}{2} A \nabla\eta \cdot \nabla\eta \quad (78)$$

where  $\beta = \rho C / 2\theta_0$  as usual. As a result, we obtain

$$\theta = \frac{\partial\epsilon}{\partial\eta} + \frac{\alpha}{\rho} \dot{\eta} - \frac{A}{\rho} \nabla^2 \eta \quad (79)$$

to be inserted in the new form of heat equation in the presence of a viscous generalized stress  $a^v$ :

$$(\rho\theta - a^v)\dot{\eta} = -\text{div} \underline{\mathbf{q}} \quad (80)$$

Taking the constitutive equation,  $a^v = \alpha\dot{\eta}$ , into account, it turns out that the contribution  $a^v \dot{\eta}$  is nonlinear so that it can be neglected. We finally obtain the following linearized generalized heat equation:

$$\rho\theta_0\dot{\eta} = \kappa \nabla^2 \theta = \kappa \left( \frac{\rho}{2\beta} \nabla^2 \eta + \frac{\alpha}{\rho} \nabla^2 \dot{\eta} - \frac{A}{\rho} \nabla^4 \eta \right) \quad (81)$$

When  $\alpha = 0$ , the latter equation is a Cahn–Hilliard type equation for heat conduction, as derived earlier (Forest and Amestoy, 2008). In the general case, the partial differential operator in Eq. (81) is the same as in (51), according to the double temperature theory, with the exception of the double time derivative.

The leading terms in (81) can be expressed as functions of the temperature variable using the state law (79) and its further derivatives:

$$\dot{\eta} = \frac{C}{\theta_0} \dot{\theta} - \frac{C\alpha}{\rho\theta_0} \ddot{\eta} + \frac{CA}{\rho\theta_0} \nabla^2 \dot{\eta} \quad (82)$$

$$\ddot{\eta} = \frac{C}{\theta_0} \ddot{\theta} - \frac{C\alpha}{\rho\theta_0} \ddot{\eta} + \frac{CA}{\rho\theta_0} \nabla^2 \ddot{\eta} \quad (83)$$

$$\nabla^2 \dot{\eta} = \frac{C}{\theta_0} \nabla^2 \dot{\theta} - \frac{C\alpha}{\rho\theta_0} \nabla^2 \ddot{\eta} + \frac{CA}{\rho\theta_0} \nabla^4 \dot{\eta} \quad (84)$$

The generalized heat equation can be rewritten in the form:

$$\rho C \dot{\theta} - \frac{C^2 \alpha}{\theta_0} \ddot{\theta} = \kappa \nabla^2 \theta - \frac{C^2 A}{\theta_0} \nabla^2 \dot{\theta} - \frac{C^2 \alpha^2}{\rho \theta_0} \ddot{\eta} + 2 \frac{C^2 \alpha A}{\rho \theta_0} \nabla^2 \ddot{\eta} - \frac{C^2 A^2}{\rho \theta_0} \nabla^4 \dot{\eta} \quad (85)$$

This equation differs from the one found within the framework of the gradient of temperature theory, Eq. (69). This proves that the gradient of entropy and gradient of temperature are distinct models. This is in contrast to the classical theory for which temperature and entropy are strictly dual variables. However, the leading terms in Eq. (85) are the same as in Eq. (69). The correction terms, proportional to  $A^2, A\alpha$  and  $\alpha^2$ , include higher order time and space derivatives of the entropy. Note that the sign of the coefficient in front of  $\ddot{\theta}$  is the same as in Eq. (69), and therefore different from the Eq. (51) when  $h > 0$ .



### 3.3. Micro-entropy

If one strictly follows the micromorphic approach sketched in Section 2.2 for plasticity, one should extend the usual thermomechanics, characterized by the sets,

$$DOFO = \{\underline{\mathbf{u}}, \theta\}, \quad STATEO = \{\underline{\boldsymbol{\varepsilon}}^e, \theta, \alpha\} \quad (86)$$

by introducing a micro-temperature variable  ${}^z\theta$ , independent of  $\theta$ , and looking for the influence of its gradient  $\nabla {}^z\theta$ :

$$DOF = \{\underline{\mathbf{u}}, \theta, {}^z\theta\}, \quad STATE = \{\underline{\boldsymbol{\varepsilon}}^e, \theta, \alpha, {}^z\theta, \nabla {}^z\theta\} \quad (87)$$

We are equally entitled to introduce a micro-entropy variable  ${}^z\eta$ , instead of the micro-temperature. The preference for the choice of the entropy variable has been motivated at the beginning of Section 3.2.2. Furthermore, we concentrate on the purely thermal case, so that:

$$DOF = \{\eta, {}^z\eta\}, \quad STATE = \{\eta, {}^z\eta, \nabla {}^z\eta\} \quad (88)$$

Within the micromorphic approach, there exists an additional independent power expenditure due to  ${}^z\dot{\eta}$ ,  $\nabla {}^z\dot{\eta}$ :

$$p^{(i)} = a {}^z\dot{\eta} + \underline{\mathbf{b}} \cdot \nabla {}^z\dot{\eta}, \quad p^{(c)} = a^c {}^z\dot{\eta} \quad (89)$$

that leads to the additional balance Eq. (56), with the associated boundary conditions. Assuming the functional dependence  $\epsilon(\eta, {}^z\eta, \nabla {}^z\eta)$ , the Clausius–Duhem inequality takes the form

$$\rho \left( \theta - \frac{\partial \epsilon}{\partial \eta} \right) \dot{\eta} + \left( a - \rho \frac{\partial \epsilon}{\partial {}^z\eta} \right) {}^z\dot{\eta} + \left( \underline{\mathbf{b}} - \rho \frac{\partial \psi}{\partial \nabla {}^z\eta} \right) \cdot \nabla {}^z\dot{\eta} - \underline{\mathbf{q}} \cdot \frac{\nabla \theta}{\theta} \geq 0 \quad (90)$$

The following state equations are adopted:

$$\theta = \frac{\partial \epsilon}{\partial \eta}, \quad a = \rho \frac{\partial \epsilon}{\partial {}^z\eta}, \quad \underline{\mathbf{b}} = \rho \frac{\partial \psi}{\partial \nabla {}^z\eta} \quad (91)$$

Within a linear context, the following quadratic potential is proposed:

$$\rho \epsilon(\eta, {}^z\eta, \nabla {}^z\eta) = \rho \eta \theta_0 + \frac{\rho^2 (\eta - \eta_0)^2}{4\beta} + \frac{1}{2} {}^zH (\eta - {}^z\eta)^2 + \frac{1}{2} A \nabla {}^z\eta \cdot \nabla {}^z\eta \quad (92)$$

In comparison to Eq. (78), a parameter  ${}^zH$  has been added in order to penalize the difference between micro and macro-entropy. It follows that

$$\theta = \theta_0 + \frac{\rho}{2\beta} (\eta - \eta_0) + \frac{{}^zH}{\rho} (\eta - {}^z\eta), \\ a = -{}^zH (\eta - {}^z\eta), \quad \underline{\mathbf{b}} = A \nabla {}^z\eta \quad (93)$$

Combining then the heat Eq. (62), the relevant state equations and the balance Eq. (56), the following generalized heat equation is obtained:

$$\rho \theta_0 \dot{\eta} = \kappa \left( \frac{\rho}{2\beta} \nabla^2 \eta - \frac{A}{\rho} \nabla^4 {}^z\eta \right) \quad (94)$$

This equation coincides with the result given by Eq. (81) of the gradient of entropy theory, specialized for  $\alpha = 0$ , when the following internal constraint is enforced:

$${}^z\eta \equiv \eta \quad (95)$$

Such a condition is almost exactly satisfied when the penalty factor  ${}^zH$  becomes sufficiently high. For a strict respect of the internal constraint, a Lagrange multiplier must be introduced. As a result, the gradient of entropy theory can be regarded as a limit case of the micro-entropy model.

### 4. Conclusions

The main conclusions of this work are the following:

- Aifantis gradient elasticity was derived from Mindlin's strain gradient linear isotropic elasticity theory, based on a specific constitutive assumption that aims at limiting the number of higher order elastic moduli. At the same time, this assumption leads to a good description of a number of experimental results and observations, in a robust manner which could not be interpreted by classical elasticity or would be very difficult to address with more complex generalized theories. This choice remains however specific and other simplifications can be preferable in other possible circumstances. When the higher order moduli are derived from a homogenization procedure for heterogeneous materials, the need for such a simplification may be mediated and all Mindlin's higher order moduli may be computed, as done for instance in Boutin (1996).
- Eringen's micromorphic theory is based on the introduction of additional microdeformation degrees of freedom. This approach can be applied to constitutive quantities other than the total strain. As an example, a plastic microstrain has been introduced in this work, together with a specific quadratic free energy potential containing the difference between micro and macro plastic strain, and the effect of the gradient of plastic micro-strain. Aifantis gradient plasticity model has been shown to arise when a well-suited internal constraint is enforced in this micromorphic model.
- Generalized stresses have also been assigned to temperature and entropy rates, and their gradients, in order to derive higher order heat equations. This approach, akin to Gurtin's microforce framework applied to mass diffusion, delivers contributions closely related to Cattaneo equations and their generalization. The same theory has been obtained also as a limiting case of a micromorphic theory of heat, involving a micro-entropy degree of freedom.
- A dissipative contribution has been incorporated in the gradient of entropy theory of Forest and Amestoy (2008) and has been shown to provide a double time derivative of temperature in the heat equation, in addition to the mixed time and space derivative term. However the sign of the corresponding coefficient differs from that in Cattaneo's equation. This fact may set the limits of the proposed gradient of entropy/temperature approach, giving advantage to the double temperature mixture theory. However, the question remains open since temperature field measurements and identifications of the parameters from extreme experiments like thermal treatment with femtosecond lasers, remain seldom so that it is not possible to conclude yet that Cattaneo's equation is, in any case, the best-suited form. Also the new contributions to the heat equations differ in the gradient of temperature model and in the gradient of entropy theory, which cannot be regarded as dual theories any more. There exist alternative approaches to Gurtin's treatment. For instance, an entropy source term is added in the second principle by Irempan and Nguyen (2004), Nguyen (2010) and leads to a generalized heat equation that differs from both (52) and (69) but also removes the paradox of instantaneous propagation of heat.
- The most general forms of extended heat equations are that delivered by the double temperature model and by the gradient of entropy model. They involve a fourth order space derivative and mixed time and space derivatives of temperature and entropy respectively.

One main advantage of the micromorphic approach compared to strain gradient or gradient of internal variable model lies in

the rather straightforward numerical implementation (Engelen et al., 2003). The additional degrees of freedom are kinematically independent, even though they are constitutively coupled. In particular, when a plastic microstrain  $\chi_p$  is introduced in addition to  $p$ , there is no need for an elastic–plastic front-tracking method as usually needed in finite element simulations with gradient models (Liebe et al., 2003). The gradient model can be obtained from the micromorphic one by introducing additional Lagrange multipliers. On the other hand, the gradient theory approach is physically-based and the various gradient terms may be motivated by the underlying mechanisms and related microstructural observations. More recently an averaging procedure for connecting macro to micro fields has been used in Aifantis (2009b) to obtain higher order differential equations for elasticity and diffusion on the basis of the standard differential equations that govern classical elasticity and mass transport processes. In a sense this procedure is reminiscent of the present micromorphic approach but it is not as rigorous and systematic as the proposed one here and in relation to the extra boundary condition required.

The micromorphic approach has already been applied to the mass diffusion equation (Forest, 2008) by introducing the micro-concentration variable, akin to the micro-entropy variable used in the present work. It was shown that the constrained micro-concentration theory coincides with the Cahn–Hilliard diffusion model. In a similar way, we have shown here that the micro-entropy model converges toward the hyper-entropy theory, when the internal constraint that the micro-entropy coincides with the macro-entropy variable, is enforced.

A unifying framework seems to emerge for classifying “higher grade” and “higher order” purely mechanical continuum theories. Coupling with other phenomena can be performed in a systematic way by means of the method of virtual power and of continuum thermomechanics, e.g. (Maugin, 1980). However, the picture is quite different concerning generalized heat or mass diffusion equations, since the signs of the coefficient in front of the additional terms remain to be discussed, for instance based on physical microstructural arguments, but also regarding uniqueness and stability of solutions of the relevant partial differential equations.

Most existing applications of generalized heat equations only incorporate a characteristic time associated with Cattaneo’s second time derivative of temperature, or with the double temperature model when one phase is far much conductive than the other one. More sophisticated simulations will be necessary to evaluate the relevance of the various higher order time and space derivatives put forward in this work, in relation to currently growing experimental facts, like the size of heat affected zones in laser treated metals. Although we are not able in the present state to give physical reasons for preferring Eq. (51) or (81), these generalized heat equations and their method of derivation can be useful in the current discussion of the use of generalized heat equations in microfluidics or laser surface treatment applications.

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