

INTERNAL STRUCTURES AND INTERNAL VARIABLES IN SOLIDS

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ABSTRACT. The response of many materials (metals, alloys, composites, etc) to external loading may be essentially influenced by an existing or emerging internal structure at smaller scales which must be taken into account. For this purpose the concept of dual internal variables can be used in order to describe the effect of internal fields. In this paper it is shown that the dual internal variable theory is sufficiently general to model cases like the micromorphic elasticity and the influence of microtemperature. Based on the material (canonical) balance equations for material momentum and energy, this approach extends the single internal variable theory. The resulting governing equations are not limited by first-order reaction-diffusion equations, as it is typical for the single internal variable theory. Hyperbolic governing equations for internal variables provide the description of the interaction of waves at macro- and micro-levels.

1. INTRODUCTION

The observed complexity in the dynamic behaviour of solids is due to the fact that solids are inherently microstructured. *Internal structures* appear at different length scales and often coexist at more than one length scale within the same solid. The description of the microstructure influence on the macromotion is therefore a necessary step for both theory and practice. However, as it is pointed out [Kirchner and Steinmann 2005], "there is no unique answer to the question how the microstructure influence can be accounted for in a continuum mechanical model". In general terms, microstructures in elastic solids can be either natural or man-made. Man-made microstructures are usually completely ordered (like laminates) and then their influence can be taken into account by direct numerical computations by making use of well-defined geometry. In contrast, the influence of disordered microstructures (both natural and man-made) leads to certain internal fields, which affect the macroscopic behavior, and the modeling of these fields may be an effective way to understand the complexity of such solids.

Over the past five decades, a number of advanced generalized continuum theories have been introduced to take into account the influence of the structural inhomogeneities on the macroscopic behavior of materials (see overview in [Maugin 2011b]). The mathematical structure of such theories [Capriz 1989] includes a coarse grained morphological descriptor introduced to describe the morphology of the material element [Mariano and Stazi 2005], which represents certain additional independent fields [Mariano 2002]. For example, considering the material element as a cell able to deform independently of the rest of the body, Mindlin [Mindlin 1964] in fact introduced a second order symmetric tensor as a morphological descriptor. The relevant continuum theory is called micromorphic [Eringen and Suhubi 1964].

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Recently, it is found that the time evolution laws for the averaged conserved dynamical variables derived from a molecular dynamic model follow exactly the balance laws in a micromorphic continuum [Chen and Lee 2003a]. Moreover, a multiscale field theory has been constructed for the concurrent atomic-continuum modeling of materials [Chen and Lee 2005, Chen and Lee 2006]. The micromorphic theory is thus considered as the most successful top-down formulation of a two-level continuum model, in which the deformation is composed of the macroscopic continuous deformation and the internal microscopic deformation of the inner structure [Hirschberger, Kuhl and Steinmann 2007, Grammenoudis and Tsakmakis 2009, Forest 2009, Wang and Lee 2010, Gonella, Greene and Liu 2011].

Alternatively, one can introduce *internal variables* to describe microstructural effects. Application of internal variables to the description of microstructural influence on global motion has a long history. As it is pointed out [Truesdell 1984], Duhem was the first who introduced what are now called internal state variables. In 1940s, Bridgman proposed an introduction of “a large scale thermodynamic parameter of state” [Bridgman 1943], which extends the state space. The thermodynamic theory of internal variables [Coleman and Gurtin 1967] had presupposed only first-order evolution equations for the internal variables and did not include their gradients. Accounting for the gradients leads to the weakly nonlocal theory [Maugin and Muschik 1994, Maugin 1999], which can be also enriched by the extra entropy flux [Maugin 1990]. The comprehensive theory of the internal state variables is presented recently [Maugin 2006].

Internal variables are usually responsible for dissipative processes and must satisfy only the second law of thermodynamics. It is hoped that a few aggregate internal variables will adequately describe the influence of a microstructure [Rice 1971, Muschik 1990, Maugin and Muschik 1994]. However, as it is noted by [Kirchner and Steinmann 2005], “it is neither a priori known which specific features of the microstructure characterize such a macroscopic internal variable, nor whether the macroscopic behavior is described sufficiently accurately by such a quantity”.

At the same time, the recently developed concept of dual internal variables [Ván et al. 2008] permits to retrieve the Mindlin micromorphic theory [Berezovski et al. 2011a] on the basis of the material formulation of continuum mechanics [Maugin 1993, Maugin 2011a]. This means that the dual internal variable approach is at least as powerful as the widely accepted micromorphic description. The material formulation takes internal variables into account naturally and consistently. Moreover, the structure of the governing equations for the microfields ensues directly from the Clausius-Duhem inequality, and not considered as granted like it is in the multifields theories [Capriz 1989] or derived from the requirement of invariance of the external power actions [Mariano 2002].

It is noted that the question how thermal effects should be taken into account in higher-order theories need further analysis [Forest and Aifantis 2010]. In the developed dual internal variable theory temperature effects can be included consistently [Berezovski et al. 2011b].

The objective of the present paper is to demonstrate how different models of *internal structure* are related to a systematic thermomechanical method of the description of *internal fields* in solids, that we call the *dual internal variables* approach. This theory is the direct extension of the comprehensive single internal variable theory [Maugin 2006]. The theory is presented here in the tensorial form generalizing preliminary results in one-dimensional setting [Berezovski et al. 2009a, Berezovski et al. 2009b].

2. THERMOMECHANICS WITH DUAL INTERNAL VARIABLES

2A. Piola-Kirchhoff formulation. The starting point in the formulation of the thermomechanics with dual internal variables is the standard continuum mechanics. To formulate the balance laws of continuum mechanics, we consider the motion of a body as a time-parametrized mapping χ , which connects a material point \mathbf{X} in the reference configuration and its position \mathbf{x} in the actual configuration in Euclidean physical space,

$$\mathbf{x} = \chi(\mathbf{X}, t). \quad (2-1)$$

Accordingly, the deformation gradient is defined by

$$\mathbf{F} = \left. \frac{\partial \chi}{\partial \mathbf{X}} \right|_t = \nabla_{R\chi}. \quad (2-2)$$

At any regular material point \mathbf{X} in a continuous body in the presence of a body force \mathbf{f}_0 per unit reference volume, the local balance laws in the so-called Piola-Kirchhoff formulation include (cf. [Wang and Truesdell 1973, Maugin 1993, Maugin 2011a]) the mass conservation

$$\left. \frac{\partial \rho_0}{\partial t} \right|_{\mathbf{x}} = 0, \quad (2-3)$$

the balance of linear momentum

$$\left. \frac{\partial(\rho_0 \mathbf{v})}{\partial t} \right|_{\mathbf{x}} - \text{Div}_R \mathbf{T} = \mathbf{f}_0, \quad (2-4)$$

and the energy conservation equation

$$\left. \frac{\partial(K + E)}{\partial t} \right|_{\mathbf{x}} - \nabla_R \cdot (\mathbf{T} \cdot \mathbf{v} - \mathbf{Q}) = \mathbf{f}_0 \cdot \mathbf{v}. \quad (2-5)$$

Balance laws (2-3)–(2-5) are complemented by the second law of thermodynamics [Maugin 1999]

$$\left. \frac{\partial S}{\partial t} \right|_{\mathbf{x}} + \nabla_R \cdot \mathbf{S} \geq 0, \quad \mathbf{S} = (\mathbf{Q}/\theta) + \mathbf{J}. \quad (2-6)$$

Here ρ_0 is the mass density in the reference configuration, $\mathbf{v} = \left. \frac{\partial \chi}{\partial t} \right|_{\mathbf{x}}$ is the physical velocity, \mathbf{T} is the first Piola-Kirchhoff stress tensor, $K = \frac{1}{2} \rho_0 \mathbf{v}^2$ is the kinetic energy per unit reference volume, E is the internal energy per unit reference volume, \mathbf{Q} is the material heat flux, S is the entropy density per unit reference volume, θ is the absolute temperature, \mathbf{S} is the entropy flux, and the "extra entropy flux" \mathbf{J} vanishes in most cases, but this is not a basic requirement, $\frac{d}{dt} = \left. \frac{\partial}{\partial t} \right|_{\mathbf{x}}$ or a superimposed dot denotes the material time derivative.

2B. Material (canonical) formulation. It is well known that balance laws (2-4)–(2-5) can be represented in the so-called material (canonical) formulation [Maugin 1993, Maugin 2011a]. The canonical form of the energy conservation for sufficiently smooth fields at any regular material point \mathbf{X} in the body has the form [Maugin 2006, Maugin and Berezovski 2008]

$$\left. \frac{\partial(S\theta)}{\partial t} \right|_{\mathbf{x}} + \nabla_R \cdot \mathbf{Q} = h^{int}, \quad h^{int} := \mathbf{T} : \dot{\mathbf{F}} - \left. \frac{\partial W}{\partial t} \right|_{\mathbf{x}}. \quad (2-7)$$

Here $W = E - \theta S$ is the Helmholtz free energy function.

Correspondingly, the canonical (material) momentum balance equation in the presence of a body force \mathbf{f}_0 per unit reference volume is written as [Maugin 2006, Maugin and Berezovski 2008]

$$\left. \frac{\partial \mathbf{P}}{\partial t} \right|_{\mathbf{X}} - \text{Div}_R \mathbf{b} = \mathbf{f}^{int} + \mathbf{f}^{ext} + \mathbf{f}^{inh}, \quad (2-8)$$

where the *material momentum* \mathbf{P} , the material *Eshelby stress* \mathbf{b} , the material *inhomogeneity force* \mathbf{f}^{inh} , the material *external* (or body) force \mathbf{f}^{ext} , and the material *internal force* \mathbf{f}^{int} are defined by

$$\mathbf{P} := -\rho_0 \mathbf{v} \cdot \mathbf{F}, \quad \mathbf{b} = -(\mathbf{L}\mathbf{I}_R + \mathbf{T}\cdot\mathbf{F}), \quad L = K - W, \quad (2-9)$$

$$\mathbf{f}^{inh} := \left. \frac{\partial L}{\partial \mathbf{X}} \right|_{expl} \equiv \left. \frac{\partial L}{\partial \mathbf{X}} \right|_{fixed\ fields} = \left(\frac{1}{2} \mathbf{v}^2 \right) \nabla_R \rho_0 - \left. \frac{\partial W}{\partial \mathbf{X}} \right|_{expl}, \quad (2-10)$$

$$\mathbf{f}^{ext} := -\mathbf{f}_0 \cdot \mathbf{F}, \quad \mathbf{f}^{int} = \mathbf{T} : (\nabla_R \mathbf{F})^T - \nabla_R W|_{impl}. \quad (2-11)$$

Here the subscript notations *expl* and *impl* mean, respectively, the material gradient keeping the fields fixed (and thus extracting the explicit dependence on \mathbf{X}), and taking the material gradient only through the fields present in the function, the "dot" notation is used for the product of two tensors.

The second law (2-6) multiplied by θ yields the Clausius-Duhem inequality

$$- \left(\frac{\partial W}{\partial t} + S \frac{\partial \theta}{\partial t} \right) \Big|_{\mathbf{X}} + \mathbf{T} : \dot{\mathbf{F}} + \nabla_R \cdot (\theta \mathbf{J}) - \mathbf{S} \cdot \nabla_R \theta \geq 0. \quad (2-12)$$

Canonical equations (2-7) and (2-8) are the most general equations for momentum and energy we can write down without a specification of the full dependency of free energy [Maugin 2006, Maugin and Berezovski 2008, Maugin 2011a]. These equations provide the basis of the description of a microstructured medium by means of the introduction of additional internal fields.

2C. Dual internal variables. The role of internal variables in continuum mechanics is described [Maugin 1990, Maugin and Muschik 1994, Maugin 2006] bearing in mind dissipative processes. As it was shown [Ván et al. 2008], an unified treatment of both dissipative and non-dissipative internal processes is possible in the framework of *dual* internal variables theory. This approach is an extension of the classical single internal variable theory. Moreover, the limitation of governing equations to first-order ones only is avoided by the concept of dual internal variables [Ván et al. 2008]. In what follows, the application of the dual internal variables to thermomechanics [Berezovski et al. 2011a] is reminded shortly.

Thus, in the framework of the phenomenological continuum theory, it is assumed that the influence of a microstructure on the overall macroscopic motion of a body can be taken into account by the introduction of internal variables, which we associate with the integral distributed effect of the microstructure. The free energy W depends (in addition to the deformation gradient and temperature) on two internal variables, $\boldsymbol{\alpha}$ and $\boldsymbol{\beta}$, each of which is a second-order tensor, and their gradients

$$W = \overline{W}(\mathbf{F}, \theta, \boldsymbol{\alpha}, \nabla_R \boldsymbol{\alpha}, \boldsymbol{\beta}, \nabla_R \boldsymbol{\beta}). \quad (2-13)$$

The inclusion of gradients into the state space is related to a weak non-locality of the theory. In this case, the equations of state are given by

$$\begin{aligned} \mathbf{T} &= \frac{\partial \overline{W}}{\partial \mathbf{F}}, \quad S = -\frac{\partial \overline{W}}{\partial \theta}, \quad \mathbf{A} := -\frac{\partial \overline{W}}{\partial \boldsymbol{\alpha}}, \quad \mathcal{A} := -\frac{\partial \overline{W}}{\partial \nabla_R \boldsymbol{\alpha}}, \\ \mathbf{B} &:= -\frac{\partial \overline{W}}{\partial \boldsymbol{\beta}}, \quad \mathcal{B} := -\frac{\partial \overline{W}}{\partial \nabla_R \boldsymbol{\beta}}. \end{aligned} \quad (2-14)$$

The main advantage of the material formulation of continuum mechanics is that the canonical equations of momentum and energy keep their form [Berezovski et al. 2011a]

$$\begin{aligned} \left. \frac{\partial \mathbf{P}}{\partial t} \right|_{\mathbf{x}} - \text{Div}_R \tilde{\mathbf{b}} &= \mathbf{f}^{th} + \tilde{\mathbf{f}}^{intr}, \\ \left. \frac{\partial(S\theta)}{\partial t} \right|_{\mathbf{x}} + \nabla_R \cdot \tilde{\mathbf{Q}} &= h^{th} + \tilde{h}^{intr}, \end{aligned} \quad (2-15)$$

with the modified Eshelby stress tensor

$$\tilde{\mathbf{b}} = -(L\mathbf{1}_R + \mathbf{T} \cdot \mathbf{F} - \mathcal{A} : (\nabla_R \boldsymbol{\alpha})^T - \mathcal{B} : (\nabla_R \boldsymbol{\beta})^T), \quad (2-16)$$

thermal source terms

$$\mathbf{f}^{th} = S \nabla_R \theta, \quad h^{th} = S \dot{\theta}, \quad (2-17)$$

and intrinsic source terms

$$\tilde{\mathbf{f}}^{intr} := \tilde{\mathcal{A}} : \nabla_R \boldsymbol{\alpha} + \tilde{\mathcal{B}} : \nabla_R \boldsymbol{\beta}, \quad \tilde{h}^{intr} := \tilde{\mathcal{A}} : \dot{\boldsymbol{\alpha}} + \tilde{\mathcal{B}} : \dot{\boldsymbol{\beta}}. \quad (2-18)$$

In the above equations the following definitions are used

$$\tilde{\mathcal{A}} := - \left(\frac{\partial \bar{W}}{\partial \boldsymbol{\alpha}} - \text{Div}_R \frac{\partial \bar{W}}{\partial (\nabla_R \boldsymbol{\alpha})} \right) = \mathbf{A} - \text{Div}_R \mathcal{A}, \quad (2-19)$$

$$\tilde{\mathcal{B}} := - \left(\frac{\partial \bar{W}}{\partial \boldsymbol{\beta}} - \text{Div}_R \frac{\partial \bar{W}}{\partial (\nabla_R \boldsymbol{\beta})} \right) = \mathbf{B} - \text{Div}_R \mathcal{B}, \quad (2-20)$$

$$\tilde{\mathbf{S}} = \theta^{-1} \tilde{\mathbf{Q}}, \quad \tilde{\mathbf{Q}} = \mathbf{Q} - \mathcal{A} : \dot{\boldsymbol{\alpha}} - \mathcal{B} : \dot{\boldsymbol{\beta}}. \quad (2-21)$$

In this formulation the Eshelby stress complies with its role of grasping all effects presenting gradients since the material gradients of internal variables play a role parallel to that of the deformation gradient \mathbf{F} .

2D. Governing equations for internal variables. Following the scheme originally developed in [Mauguin 1990] for materials with diffusive dissipative processes described by means of internal variables of state, we chose the non-zero extra entropy flux in the form

$$\mathbf{J} = -\theta^{-1} \mathcal{A} : \dot{\boldsymbol{\alpha}} - \theta^{-1} \mathcal{B} : \dot{\boldsymbol{\beta}}. \quad (2-22)$$

Dissipation inequality (2-12) is then reduced to

$$\Phi = \tilde{\mathcal{A}} : \dot{\boldsymbol{\alpha}} + \tilde{\mathcal{B}} : \dot{\boldsymbol{\beta}} - \tilde{\mathbf{S}} \nabla_R \theta \geq 0, \quad (2-23)$$

and contains both intrinsic and thermal parts. The thermal part of this inequality can be satisfied by the modification of the Fourier law [Berezovski et al. 2011b], which is nothing else but the standard proportionality of the heat flux with respect to the temperature gradient

$$\mathbf{Q} - \mathcal{A} : \dot{\boldsymbol{\alpha}} - \mathcal{B} : \dot{\boldsymbol{\beta}} = -a^2 \nabla_R \theta. \quad (2-24)$$

The intrinsic part of dissipation inequality (2-23) depends solely on internal fields

$$\tilde{h}^{intr} := \tilde{\mathcal{A}} : \dot{\boldsymbol{\alpha}} + \tilde{\mathcal{B}} : \dot{\boldsymbol{\beta}} \geq 0. \quad (2-25)$$

The governing equations for the internal variables $\boldsymbol{\alpha}$ and $\boldsymbol{\beta}$ yield from Eq. (2-25) as follows

$$\begin{pmatrix} \dot{\boldsymbol{\alpha}} \\ \dot{\boldsymbol{\beta}} \end{pmatrix} = \mathbf{R} \begin{pmatrix} \tilde{\mathcal{A}} \\ \tilde{\mathcal{B}} \end{pmatrix}, \quad \text{or} \quad \begin{pmatrix} \dot{\boldsymbol{\alpha}} \\ \dot{\boldsymbol{\beta}} \end{pmatrix} = \begin{pmatrix} \mathbf{R}^{11} & \mathbf{R}^{12} \\ \mathbf{R}^{21} & \mathbf{R}^{22} \end{pmatrix} \begin{pmatrix} \tilde{\mathcal{A}} \\ \tilde{\mathcal{B}} \end{pmatrix}, \quad (2-26)$$

where components $\mathbf{R}^{11}, \dots, \mathbf{R}^{22}$ of the linear operator \mathbf{R} are dependent on state variables [Gurtin 1996].

2E. Remarks. The governing equations for the internal variables (2-26) complete the basic theory of the thermomechanics with dual internal variables. Formally, this theory is the direct extension of the comprehensive single internal variable theory [Maugin 2006]. This is a weakly non-local theory in the material formulation enriched by the extra entropy flux similarly to that in the single internal variable theory [Ván et al. 2008]. However, the introduction of the additional internal variables may change the mathematical structure of the theory. As it was demonstrated [Berezovski et al. 2011b], in addition to the dissipative part, the dual internal variables contribute also into the reversible Poisson structure [Mielke 2011]. This is the origin of hyperbolic governing equations for the dual internal variables that generalizes the internal variable theory significantly.

The given formulation of the theory is certainly of a general character and should be specified to describe a particular influence of an internal structure. We will demonstrate the ability of the theory on certain examples focussing on the explicit form of governing equations for the internal variables. The governing equations coupled with the balance of momentum and energy constitute the corresponding continuum model with the influence of internal structure. Though each particular case is characterized by an explicit form of the free energy, we will keep the free energy as general as possible.

3. EXAMPLE 1: PURE DISSIPATIVE CASE

Representing the linear operator \mathbf{R} as the sum of symmetric and skew-symmetric components $\mathbf{R} = (\mathbf{R} + \mathbf{R}^T)/2 + (\mathbf{R} - \mathbf{R}^T)/2$, i.e.,

$$\begin{pmatrix} \dot{\boldsymbol{\alpha}} \\ \dot{\boldsymbol{\beta}} \end{pmatrix} = \begin{pmatrix} \mathbf{R}^{11} & (\mathbf{R}^{12} + \mathbf{R}^{21})/2 \\ (\mathbf{R}^{21} + \mathbf{R}^{12})/2 & \mathbf{R}^{22} \end{pmatrix} \begin{pmatrix} \tilde{\mathcal{A}} \\ \tilde{\mathcal{B}} \end{pmatrix} + \begin{pmatrix} 0 & (\mathbf{R}^{12} - \mathbf{R}^{21})/2 \\ (\mathbf{R}^{21} - \mathbf{R}^{12})/2 & 0 \end{pmatrix} \begin{pmatrix} \tilde{\mathcal{A}} \\ \tilde{\mathcal{B}} \end{pmatrix}, \quad (3-1)$$

we can see that the symmetry of the linear operator \mathbf{R} , which is equivalent to the Onsagerian reciprocity relations $\mathbf{R}^{12} = \mathbf{R}^{21}$, leads to the elimination of the antisymmetric part of the linear operator \mathbf{R} . In this case, we return to the classical situation, where internal variables are fully independent, dissipative, and governed by reaction-diffusion equations [Coleman and Gurtin 1967, Maugin and Muschik 1994, Maugin 2006].

In fact, the governing equations for the internal variables in this case

$$\dot{\boldsymbol{\alpha}} = \mathbf{R}^{11} \cdot \tilde{\mathcal{A}}, \quad \dot{\boldsymbol{\beta}} = \mathbf{R}^{22} \cdot \tilde{\mathcal{B}}, \quad (3-2)$$

automatically provide the non-negativity of the intrinsic part of dissipation inequality (2-25)

$$\tilde{h}^{intr} := \tilde{\mathcal{A}} : \dot{\boldsymbol{\alpha}} + \tilde{\mathcal{B}} : \dot{\boldsymbol{\beta}} \geq 0, \quad (3-3)$$

if \mathbf{R}^{11} and \mathbf{R}^{22} are positive definite. Obtained reaction-diffusion-like equations

$$\dot{\boldsymbol{\alpha}} = \mathbf{R}^{11} \cdot (\mathbf{A} - Div_R \mathcal{A}), \quad \text{or} \quad \dot{\boldsymbol{\beta}} = \mathbf{R}^{22} \cdot (\mathbf{B} - Div_R \mathcal{B}), \quad (3-4)$$

can be found under different names in numerous applications. For example, if the free energy depends on a scalar internal variable α as

$$W = \bar{W}(\dots, \alpha, \nabla_R \alpha) = f(\dots, \alpha) + \frac{1}{2} D(\nabla \alpha)^2, \quad (3-5)$$

we arrive at the Ginzburg-Landau (or the Allen-Cahn) equation (cf. [Cross and Hohenberg 1993])

$$\frac{1}{k}\dot{\alpha} = D\nabla^2\alpha - f'(\alpha), \quad (3-6)$$

where $f'(\alpha)$ denotes the derivative with respect to α .

As we can conclude, the single internal variable theory is a particular case of the theory with dual internal variables. In the case of a pure dissipative internal structure, there is no need to go beyond the single internal variable theory. However, we have no reasons to assume the symmetry of the linear operator \mathbf{R} in the case of arbitrary internal structures.

4. EXAMPLE 2: PURE NON-DISSIPATIVE CASE

The pure non-dissipative case corresponds to the skew-symmetric matrix \mathbf{R} , which implies $\mathbf{R}^{11} = \mathbf{R}^{22} = \mathbf{0}$ and the Casimirian reciprocity relations $\mathbf{R}^{12} = -\mathbf{R}^{21}$. The governing equations for the dual internal variables are fully coupled

$$\dot{\alpha} = \mathbf{R}^{12}.\tilde{\mathcal{B}} = \mathbf{R}^{12}.\mathbf{B} - Div_R\mathcal{B}, \quad (4-1)$$

$$\dot{\beta} = -\mathbf{R}^{12}.\tilde{\mathcal{A}} = -\mathbf{R}^{12}.\mathbf{A} - Div_R\mathcal{A}, \quad (4-2)$$

and the dissipation \tilde{h}^{intr} vanishes. In this case, the evolution of one internal variable is driven by another one that manifests the duality between the internal variables.

To be more specific, let us consider a simple case with $\mathcal{B} = \mathbf{0}$, which means that the free energy function \bar{W} is independent of $\nabla_R\mathcal{B}$. Then governing equation for the first internal variable (4-1) is reduced to

$$\dot{\alpha} = \mathbf{R}^{12}.\mathbf{B}. \quad (4-3)$$

Assuming further a quadratic dependence of the free energy function with respect to the internal variable β

$$\mathbf{B} := -\frac{\partial\bar{W}}{\partial\beta} = -b\beta, \quad (4-4)$$

we reduce Eq. (4-3) even more

$$\dot{\alpha} = -b\mathbf{R}^{12}.\beta. \quad (4-5)$$

Substituting from Eq. (4-5) into Eq. (4-2), we arrive at a hyperbolic governing equation for the primary internal variable α :

$$\ddot{\alpha} = (b\mathbf{R}^{12}.\mathbf{R}^{12}).\tilde{\mathcal{A}} = (b\mathbf{R}^{12}.\mathbf{R}^{12}).\left(-\frac{\partial\bar{W}}{\partial\alpha} + Div_R\frac{\partial\bar{W}}{\partial(\nabla_R\alpha)}\right). \quad (4-6)$$

To exemplify the latter, still sufficiently general governing equation, we need to identify the abstract primary internal variable α with a certain well-known (micro)field variable. We will demonstrate such a representation on the example of the Mindlin micromorphic theory [Mindlin 1964].

4A. Mindlin micromorphic theory. In the framework of the Mindlin micromorphic theory [Mindlin 1964], each material point is endowed with three translational degrees of freedom \mathbf{u} and a second order microdeformation tensor ψ with nine independent components. In the case of centrosymmetric, isotropic materials, the equations of motion in terms of stresses [Mindlin 1964] can be represented in the form

$$\rho\dot{\mathbf{v}} = \text{div}(\boldsymbol{\sigma} + \boldsymbol{\tau}) + \mathbf{f}, \quad (4-7)$$

$$\mathbf{I}.\ddot{\psi} = \text{div}\boldsymbol{\mu} + \boldsymbol{\tau} + \Phi, \quad (4-8)$$

where \mathbf{I} is a microinertia tensor, \mathbf{f} is the body force, and Φ is the double force per unit volume. The corresponding stress tensors, namely, the Cauchy stress $\boldsymbol{\sigma}$, the relative stress $\boldsymbol{\tau}$, and the double stress $\boldsymbol{\mu}$

$$\boldsymbol{\sigma} \equiv \frac{\partial W}{\partial \boldsymbol{\varepsilon}}, \quad \boldsymbol{\tau} \equiv \frac{\partial W}{\partial \boldsymbol{\gamma}}, \quad \boldsymbol{\mu} \equiv \frac{\partial W}{\partial \boldsymbol{\varkappa}}, \quad (4-9)$$

are defined, respectively, as derivatives of the free energy with respect to the classical strain tensor $\boldsymbol{\varepsilon}$, the relative deformation tensor $\boldsymbol{\gamma}$, and the microdeformation gradient $\boldsymbol{\varkappa}$ [Mindlin 1964], where

$$\boldsymbol{\varepsilon} \equiv \frac{1}{2} (\nabla \mathbf{u} + (\nabla \mathbf{u})^T), \quad \boldsymbol{\gamma} \equiv \nabla \mathbf{u} - \boldsymbol{\psi}, \quad \boldsymbol{\varkappa} \equiv \nabla \boldsymbol{\psi}. \quad (4-10)$$

The free energy density W is supposed to be a homogeneous, quadratic function of forty-two variables $\boldsymbol{\varepsilon}, \boldsymbol{\gamma}, \boldsymbol{\varkappa}$ [Mindlin 1964]. It should be noted that the balances of linear momentum both at micro- and at macrolevel (Eqs. (4-7) and (4-8), respectively) are introduced independently.

4B. Rearrangement. As it is shown [Berezovski et al. 2011a], the constitutive relations in the micromorphic Mindlin theory can be represented in terms of distortion $\nabla \mathbf{u}$ and microdeformation tensor $\boldsymbol{\psi}$. Accordingly, the stresses are represented as follows:

$$\boldsymbol{\sigma}' \equiv \frac{\partial W}{\partial \nabla \mathbf{u}}, \quad \boldsymbol{\tau}' \equiv \frac{\partial W}{\partial \boldsymbol{\psi}}. \quad (4-11)$$

The double stress remains unchanged. Equations of motion (4-7) and (4-8) then take on the form [Berezovski et al. 2011a]

$$\rho \dot{\mathbf{v}} = \text{div} \boldsymbol{\sigma}' + \mathbf{f}, \quad (4-12)$$

$$\mathbf{I} \cdot \ddot{\boldsymbol{\psi}} = \text{div} \boldsymbol{\mu} - \boldsymbol{\tau}' + \Phi, \quad (4-13)$$

The change of the sign in the right hand side of governing equation for the microdeformation (4-13) follows from opposite signs of $\boldsymbol{\gamma}$ and $\boldsymbol{\psi}$ (see Eq. (4-10)₂).

4C. Microdeformation tensor as an internal variable. Now we consider the microdeformation tensor $\boldsymbol{\psi}$ as an internal variable $\boldsymbol{\alpha}$ and apply the formalism developed above. The microdeformation gradient $\boldsymbol{\varkappa}$ plays the role of the gradient of the internal variable $\boldsymbol{\alpha}$, and we introduce a dual internal variable $\boldsymbol{\beta}$ in the same way as it is previously described. In the non-dissipative case, the dual internal variable $\boldsymbol{\beta}$ is auxiliary and does not affect the calculation of derivatives of free energy with respect to microdeformation and double stress. Therefore, the governing equation for the internal variable $\boldsymbol{\alpha}$ follows from Eq. (4-6)

$$\ddot{\boldsymbol{\alpha}} = (b\mathbf{R}^{12} \cdot \mathbf{R}^{12}) \cdot \left(-\frac{\partial W}{\partial \boldsymbol{\alpha}} + \text{Div} \frac{\partial W}{\partial (\nabla \boldsymbol{\alpha})} \right). \quad (4-14)$$

Identifying the internal variable $\boldsymbol{\alpha}$ with the microdeformation tensor $\boldsymbol{\psi}$, the latter governing equation takes on the form

$$(b\mathbf{R}^{12} \cdot \mathbf{R}^{12})^{-1} \cdot \ddot{\boldsymbol{\psi}} = \left(-\frac{\partial W}{\partial \boldsymbol{\psi}_{jk}} + \text{Div} \frac{\partial W}{\partial (\nabla \boldsymbol{\psi}_{jk})} \right) = \text{div} \boldsymbol{\mu} - \boldsymbol{\tau}'. \quad (4-15)$$

As one can see, governing equation for the microdeformation (4-15) is practically the same as equation of motion at the microlevel (4-13) in the rearranged Mindlin theory. The external double force cannot appear in the internal variable theory [Berezovski et al. 2011a]. It should be noted that equation of motion (4-15) is not postulated, but it follows from the dissipation inequality for the chosen functional dependence of the free energy in the considered non-dissipative case. Clearly, this approach can be applied to microstrain and micropolar theories (with corresponding changes) since they are particular cases of the micromorphic theory [Eringen 1999].

5. EXAMPLE 3: A MORE GENERAL CASE (MICROTEMPERATURE EFFECTS)

Now we consider a more complicated case, including dissipative and non-dissipative contributions. We choose the matrix \mathbf{R} in Eq. (2-26) as follows:

$$\mathbf{R} = \begin{pmatrix} 0 & \mathbf{R}^{12} \\ -\mathbf{R}^{12} & \mathbf{R}^{22} \end{pmatrix}, \quad (5-1)$$

with the Casimirian reciprocity relations. The governing equations for the dual variables are coupled

$$\dot{\boldsymbol{\alpha}} = \mathbf{R}^{12} \cdot (\mathbf{B} - \text{Div}_R \mathcal{B}), \quad (5-2)$$

$$\dot{\boldsymbol{\beta}} = -\mathbf{R}^{12} \cdot (\mathbf{A} - \text{Div}_R \mathcal{A}) + \mathbf{R}^{22} \cdot (\mathbf{B} - \text{Div}_R \mathcal{B}). \quad (5-3)$$

Here the intrinsic part of the dissipation \tilde{h}^{intr} is positive. Considering again the simple case with the free energy function \bar{W} independent of $\nabla_R \boldsymbol{\beta}$ and the quadratic dependence of the free energy function with respect to the internal variable $\boldsymbol{\beta}$, we again have for the primary internal variable

$$\dot{\boldsymbol{\alpha}} = -b\mathbf{R}^{12} \cdot \boldsymbol{\beta}. \quad (5-4)$$

Substituting from Eq. (5-4) into Eq. (5-3), we obtain the governing equation for the primary internal variable $\boldsymbol{\alpha}$:

$$\ddot{\boldsymbol{\alpha}} - \mathbf{R}^{22} \cdot (\mathbf{R}^{12})^{-1} \dot{\boldsymbol{\alpha}} = (b\mathbf{R}^{12} \cdot \mathbf{R}^{12}) \cdot \left(-\frac{\partial \bar{W}}{\partial \boldsymbol{\alpha}} + \text{Div}_R \frac{\partial \bar{W}}{\partial (\nabla_R \boldsymbol{\alpha})} \right), \quad (5-5)$$

which is a Cattaneo-Vernotte-type hyperbolic equation [Joseph and Preziosi 1989]. As it was shown by [Berezovski et al. 2011b] on the example of one-dimensional thermoelasticity, the primary internal variable $\boldsymbol{\alpha}$ can be identified in this case with the microtemperature. In this context, it is understood as a fluctuation of the macrotemperature due to the influence of the existing microstructure. Governing equation (5-5) is coupled with canonical equations (2-15), because the modified Eshelby tensor $\tilde{\mathbf{b}}$ and entropy flux $\tilde{\mathbf{S}}$ include contributions by internal variables. In fact, energy conservation equation (2-15)₂ can be represented in the form

$$\theta \left. \frac{\partial S}{\partial t} \right|_{\mathbf{x}} + \nabla_R \cdot \tilde{\mathbf{Q}} = \tilde{h}^{intr}. \quad (5-6)$$

Due to definition of entropy (2-14)₂, its time derivative can be calculated as

$$\left. \frac{\partial S}{\partial t} \right|_{\mathbf{x}} = - \left. \frac{\partial^2 W}{\partial t \partial \theta} \right|_{\mathbf{x}} = - \left. \frac{\partial^2 W}{\partial \mathbf{F} \partial \theta} \right|_{\mathbf{x}} : \dot{\mathbf{F}} - \left. \frac{\partial^2 W}{\partial \theta^2} \right|_{\mathbf{x}} \dot{\theta}, \quad (5-7)$$

because internal variables are independent of temperature. Thus energy balance equation (5-6) can be represented as

$$c\dot{\theta} + \nabla_R \cdot \tilde{\mathbf{Q}} = \theta \mathbf{M} : \dot{\mathbf{F}} + \tilde{h}^{intr}, \quad (5-8)$$

with

$$c = -\theta \left. \frac{\partial^2 W}{\partial \theta^2} \right|_{\mathbf{x}}, \quad \mathbf{M} = \left. \frac{\partial^2 W}{\partial \mathbf{F} \partial \theta} \right|_{\mathbf{x}}. \quad (5-9)$$

The final form of the heat conduction equation follows from definition of $\tilde{\mathbf{Q}}$ (2-21), modified Fourier's law (2-24), and expression for the intrinsic heat source (2-25)

$$c\dot{\theta} = \nabla_R^2 \theta + \theta \mathbf{M} : \dot{\mathbf{F}} + \tilde{\mathcal{A}} : \dot{\boldsymbol{\alpha}} + \tilde{\mathcal{B}} : \dot{\boldsymbol{\beta}}. \quad (5-10)$$

This means that the heat conduction equation is still parabolic, but coupled with the stress field and internal variables. The equation of motion is the same as in the Piola-Kirchhoff formulation

(2-4), but due to the definition of the stress in the dual internal variables theory (2-14)₁, the stress tensor may contain both thermal and internal parts depending on the constitutive relation, which is not imposed yet. The coupling between the equation of motion, energy balance (5-10), and governing equation for internal variables (5-5) may induce a wave-like propagation of the macrotemperature even in the case of a parabolic equation for the macrotemperature [Berezovski et al. 2011b]. The process of wave interaction at micro- and macro-levels can be described as follows. Microtemperature perturbations are induced by a macrodeformation due to the heterogeneity in the presence of a microstructure. These perturbations, propagating with finite speed, can induce, in turn, corresponding changes in macrotemperature. At last, the appeared changes in macrotemperature affect macrodeformations once more, and so on.

6. CONCLUSIONS AND DISCUSSION

To sum up, we have shown that the influence of the internal structure of materials under external loading can be modeled by internal fields using the concept of dual internal variables. As one can see, the dual internal variable theory is sufficiently general to comprise the micromorphic elasticity and the microtemperature influence in addition to classical single internal variable reaction-diffusion-type applications. Based on the canonical balance equations for material momentum and energy, the weakly non-local dual internal variable approach leads to governing equations for internal variables, which ensue directly from the dissipation inequality. The resulting governing equations are not limited by first-order reaction-diffusion equations, as it is typical for the single internal variable theory. Appeared hyperbolic governing equations provide the description of the interaction of waves at macro- and micro-levels. In summary, the dual internal variables approach offers an unified description of dissipative and non-dissipative internal processes in solids in the framework of continuum mechanics. In contrast to other theories, the following features should be emphasized:

- Governing equations for internal variables are ensued from the dissipation inequality and, therefore they are thermodynamically consistent.
- Governing equations for internal variables are not restricted by first-order differential equations, i.e., they may include second-order derivatives responsible for wave motion.
- Boundary conditions for internal variables are determined by zero extra entropy flux at a boundary, which is a natural condition for internal variables.

At the same time, the presented theory is not a theory of everything. It is difficult to expect that the internal variable theory will describe, for example, volume double and couple forces that may appear in the general micromorphic case, because they are external by definition. This theory cannot handle any "internal" field, which can be controlled at boundaries. Such a field should be treated as an internal degree of freedom. In the corresponding case, the balance equations for the internal field should be postulated or derived separately.

The dual internal variable theory is presented in the general framework of material formulation of continuum mechanics without specifying the small strain approximation. However, the example of non-dissipative micromorphic elasticity is presented following the original Mindlin form with the small strain approximation to demonstrate explicitly the similarity of the structure of governing equations for internal fields. The introduced microtemperature adheres the micromorphic approach [Forest and Aifantis 2010]. It can be interpreted physically as fluctuations about the mean temperature. The microtemperature itself cannot produce essential influence, but its gradients can do that [Forest and Amestoy(2008)]. The introduction of the microtemperature is accompanied by the modification of the Fourier law providing the coupling between

macrotemperature and its fluctuations. The modification of the Fourier law yields from the standard choice of the proportionality of the modified heat flux to the temperature gradient in order to satisfy the thermal part of the dissipation inequality.

As for any high-order theory, the application of the described dual internal variables theory to practical problems depends on the specification of the free energy function which involves many material constants. There are several methods to determine the material constants such as the classical homogenization [Nemat-Nasser and Hori 1993] or more recent asymptotic homogenization methods [Peerlings and Fleck 2004, Fish and Fan 2008, Pindera et al. 2009].

[Chen and Lee 2003b] proposed an approach to determine the material constants for micromorphic elastic solids through the phonon dispersion relations obtained by atomistic calculations or experimental measurements. Later, [Zeng et al. 2006] extended the approach to determine material constants in the nonlocal micromorphic theory. Similar approach is proposed [Maranganti and Sharma 2007, Jakata and Every 2008] to determine coefficients of higher order derivatives in strain-gradient elasticity. An attempt is made to solve the mathematically well-posed inverse problems for determination of material parameters for micromorphic elasticity [Janno and Engelbrecht 2011].

To be able to compare theoretical and experimental dispersion curves, the dispersive wave equations for elastic solids with internal structure were retrieved, analyzed, and unified recently [Berezovski et al. 2011]. It was also shown that for a medium consisting of more than one phase of microstructure, additional internal variables are necessary in order to describe the local deformation and yield more accurate dispersion curves [Huang and Sun 2008, Berezovski et al. 2010]. Clearly, the efforts to understand the influence of internal fields on macrobehavior lead us to better understanding of mechanics of materials.

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