INTERNAL VARIABLES AND MICROSTRUCTURED MATERIALS

Arkadi Berezovski*, Jüri Engelbrecht* & Gérard A. Maugin**
*Centre for Nonlinear Studies, Institute of Cybernetics at Tallinn University of Technology, Tallinn, Estonia
**Institut Jean Le Rond d'Alembert, Université Pierre et Marie Curie, Paris Cédex 05, France

Summary A unified framework for both dissipative and non-dissipative processes based on the canonical thermomechanics on the material manifold including weakly non-local dual internal variables enriched by an extra entropy flux is proposed for the use of internal variables in the description of the microstructure influence on the dynamic behavior of materials.

INTRODUCTION

Internal variables are used for the description of microstructure in continuous media for decades. However, their usage is constrained by dissipative processes. The non-dissipative processes are associated with internal degrees of freedom. Recent developments in the internal variable theory allow us to propose a unified framework for the description of both dissipative and non-dissipative processes under one umbrella and to clarify the structure of generalized continuum theories on the basis of the canonical thermomechanics on the material manifold including weakly non-local dual internal variables enriched by an extra entropy flux. This formalism includes both dissipative reaction-diffusion equations and second grade and second gradient theories.

CANONICAL THERMOMECHANICS WITH INTERNAL VARIABLES

Let α the internal variable of state whose tensorial nature is not specified. Then the free energy per unit volume W is specified as the general sufficiently regular function of the direct-motion deformation gradient $\mathbf{F}$, temperature θ, the internal variable, and its space gradient $W = \overline{W}(\mathbf{F}, \theta, \alpha, \nabla_R \alpha)$. The equations of state determine the first Piola-Kirchhoff stress tensor $\mathbf{T}$, the entropy per unit volume S, and the quantities A and $\mathbf{A}$ corresponding to the internal variable

$$\mathbf{T} = \frac{\partial \overline{W}}{\partial \mathbf{F}}, \quad S = -\frac{\partial \overline{W}}{\partial \theta}, \quad A := -\frac{\partial \overline{W}}{\partial \alpha}, \quad \mathbf{A} := -\frac{\partial \overline{W}}{\partial \nabla_R \alpha}. \tag{1}$$

For materials with *diffusive* dissipative processes described by means of internal variables of state it is proposed [1] that there exists a non-zero extra entropy flux $\mathbf{K} = -\theta^{-1}\mathbf{A}\dot{\alpha}$. It is shown that the canonical equations of momentum and energy read (no body force) [2]

$$\frac{d\mathbf{P}}{dt} - \nabla_R \cdot \widetilde{\mathbf{b}} = \mathbf{f}^{th} + \widetilde{\mathbf{f}}^{intr}, \quad \frac{\partial (S\theta)}{\partial t} + \nabla_R \cdot \widetilde{\mathbf{Q}} = h^{th} + \widetilde{h}^{intr}, \tag{2}$$

where we have set the *material momentum* $\mathbf{P}$, the material *Eshelby stress* $\widetilde{\mathbf{b}}$,

$$\mathbf{P} := -\rho_0 \mathbf{v} \cdot \mathbf{F}, \quad \widetilde{\mathbf{b}} = -(L\mathbf{1}_R + \mathbf{T}.\mathbf{F} - \mathbf{A}.(\nabla_R \alpha)^T), \quad L = K - W, \tag{3}$$

the material *thermal* force $\mathbf{f}^{th}$, the material *intrinsic* force $\mathbf{f}^{intr}$, and the corresponding thermal sources

$$\mathbf{f}^{th} := S\nabla_R \theta, \quad h^{th} := S\dot{\theta}, \quad \widetilde{h}^{intr} := \widetilde{A}\dot{\alpha}, \quad \widetilde{\mathbf{f}}^{intr} := \widetilde{A}\nabla_R \alpha. \tag{4}$$

Here t is time, $\rho_0(\mathbf{X})$ is the matter density in the reference configuration, $\mathbf{p} = \rho_0 \mathbf{v}$ is the linear momentum, $\mathbf{v}$ is the physical velocity, $K = \frac{1}{2}\rho_0 \mathbf{v}^2$ is the kinetic energy per unit volume in the reference configuration, $\mathbf{Q}$ is the material heat flux, and the new definitions are introduced

$$\widetilde{A} = A - \nabla_R \cdot \mathbf{A}, \quad \widetilde{\mathbf{S}} = \theta^{-1}\widetilde{\mathbf{Q}}, \quad \widetilde{\mathbf{Q}} = \mathbf{Q} - \mathbf{A}\dot{\alpha}, \tag{5}$$

In this formulation the Eshelby stress complies with its role of grasping all effects presenting gradients since the material gradient of α plays a role parallel to that of the deformation gradient $\mathbf{F}$. The canonical momentum and energy equations (2) are projections of balance laws of linear momentum and energy onto the material manifold. The second law of thermodynamics is exploited in the form of the dissipation inequality

$$\Phi = \widetilde{h}^{intr} - \widetilde{\mathbf{S}}\nabla_R \theta \geq 0. \tag{6}$$

Examples of evolution equations for internal variables

The simplest way to satisfy the dissipation inequality (6) in the absence of thermal effects is the choice of the evolution equation for the internal variable α in the form $\widetilde{A} = k\dot{\alpha}$ with $k \geq 0$ since in this case $\Phi = k\dot{\alpha}^2 \geq 0$. If the free energy depends on the internal variable as

$$W = \overline{W}(..., \alpha, \nabla_R \alpha) = f(..., \alpha) + \frac{1}{2}D(\nabla \alpha)^2, \tag{7}$$

we come to the Ginzburg-Landau (Allen-Cahn) equation or the Cahn-Hilliard equation

$$k\dot{\alpha} = D\nabla^2\alpha - f'(\alpha), \quad k\dot{\alpha} = \nabla^2(D\nabla^2\alpha - f'(\alpha)). \tag{8}$$

depending of the choice $\widetilde{A} = k\dot{\alpha}$ or $\nabla^2\widetilde{A} = k\dot{\alpha}$, respectively, for the same free energy dependence.

DUAL INTERNAL VARIABLES

The generalization of the internal variable theory to the case of two internal variables is straightforward. Let us consider the free energy W as function of two internal variables, α and β, whose tensorial nature is still not specified

$$W = \overline{W}(\mathbf{F}, \theta, \alpha, \nabla_R\alpha, \beta, \nabla_R\beta). \tag{9}$$

In this case the equations of state are given by

$$\mathbf{T} = \frac{\partial\overline{W}}{\partial\mathbf{F}}, \quad S = -\frac{\partial\overline{W}}{\partial\theta}, \quad A := -\frac{\partial\overline{W}}{\partial\alpha}, \quad \mathbf{A} := -\frac{\partial\overline{W}}{\partial\nabla_R\alpha}, \quad B := -\frac{\partial\overline{W}}{\partial\beta}, \quad \mathbf{B} := -\frac{\partial\overline{W}}{\partial\nabla_R\beta}. \tag{10}$$

We include into consideration the non-zero extra entropy flux according to the case of one internal variable $\mathbf{K} = -\theta^{-1}\mathbf{A}\dot{\alpha} - \theta^{-1}\mathbf{B}\dot{\beta}$. The canonical equations of momentum and energy keep their form and the dissipation inequality

$$\widetilde{h}^{intr} := (A - \nabla_R \cdot \mathbf{A})\dot{\alpha} + (B - \nabla_R \cdot \mathbf{B})\dot{\beta} \geq 0 \tag{11}$$

can by satisfied in the non-dissipative case by the choice

$$\dot{\alpha} = l(B - \nabla_R \cdot \mathbf{B}), \quad \dot{\beta} = -l(A - \nabla_R \cdot \mathbf{A}). \tag{12}$$

In this case, the evolution of one internal variable is driven by another one that means the duality between the internal variables. Assuming a quadratic dependence of the free energy function with respect to the internal variable β, i. e. $B = -\beta$ and $\mathbf{B} = \mathbf{0}$, we come to $\dot{\alpha} = -l\beta$, and then to an evolution equation for the internal variable α with its second-order time derivative

$$\ddot{\alpha} = l^2(A - \nabla_R \cdot \mathbf{A}). \tag{13}$$

Example of evolution equations for dual internal variables

If we consider the microdeformation tensor ψ_{ij} as an internal variable $\boldsymbol{\alpha}$, then the microdeformation gradient κ_{ijk} plays the role of the gradient of the internal variable $\boldsymbol{\alpha}$, and we can introduce a dual internal variable $\boldsymbol{\beta}$ as above. In the non-dissipative case, the evolution equation for the internal variable $\boldsymbol{\alpha}$ can be symbolically written as

$$\ddot{\boldsymbol{\alpha}} = l^2\left(-\frac{\partial\overline{W}}{\partial\boldsymbol{\alpha}} + \nabla \cdot \frac{\partial\overline{W}}{\partial(\nabla\boldsymbol{\alpha})}\right). \tag{14}$$

In terms of components of the microdeformation tensor ψ_{ij} the latter evolution equation obtains the form

$$\left(l^2\right)^{-1}_{ji}\ddot{\psi}_{ik} = \left(-\frac{\partial\overline{W}}{\partial\psi_{jk}} + \nabla \cdot \frac{\partial\overline{W}}{\partial(\nabla\psi_{jk})}\right) = \partial_i\mu_{ijk} - \tau'_{jk}, \tag{15}$$

where μ_{ijk} is the double stress and τ'_{jk} is a modified Cauchy stress. As one can see, the evolution equation for the microdeformation (15) is similar to that in the linear Mindlin theory of microstructure [3].

CONCLUSIONS

As it is demonstrated, the Mindlin micromorphic theory can be represented in terms of dual internal variables in a natural way in the framework of canonical thermomechanics [2]. The micromorphic theory is a very general one and encompass both Cosserat and second gradient theories [4].

References

[1] Maugin G.A.: Internal variables and dissipative structures. *J. Non-Equilib. Thermodyn.* **15**: 173–192, 1990.
[2] Maugin G.A.: On the thermomechanics of continuous media with diffusion and/or weak nonlocality. *Arch. Appl. Mech.* **75**: 723–738, 2006.
[3] Mindlin R.D.: Micro-structure in linear elasticity. *Arch. Rat. Mech. Anal.*, **16**: 51–78, 1964.
[4] Forest S. and Sievert R.: Elastoviscoplastic constitutive frameworks for generalized continua. *Acta Mech.* **160**: 71–111, 2003.