Internal variables associated with microstructures in solids

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In memory of Professor Gérard A. Maugin

Abstract

Application of internal variables to the description of the influence of a microstructure on the overall behavior of solids is presented and discussed. It is demonstrated on the one-dimensional example that capabilities of strain gradient models are much less than those provided by internal variables.

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1. Introduction

Solid mechanics is the well established theory for homogeneous bodies. Unfortunately, bodies are homogeneous only in the first approximation. Inhomogeneities of various size, distribution, and properties compose a microstructure in real materials. The effect of the microstructure on overall response of the body may not be necessarily small even if the length scale of the microstructure is much smaller than the length scale of the body. This is why the influence of the microstructure should be taken into account in the macroscopic material description.

The detailed description of a microstructure is beyond the framework of solid mechanics. For static problems it is often sufficient to use homogenization methods of micromechanics (Mura, 1987; Nemat-Nasser and Hori, 1993) for the determination of averaged properties of "effective" media. More sophisticated asymptotic (Chen and Fish, 2001; Awrejcewicz et al., 2012) or computational (Geers et al., 2010) homogenization methods are elaborated for dynamic and nonlinear problems. The contemporary state of the art in this direction is reviewed in (Matouš et al., 2017).

A more broad and universal description of the microstructural influence is provided by generalized continuum theories (see overview by Maugin (2011)). In these theories, material elements are equipped by certain additional independent kinematic fields like the microrotation in a Cosserat material or the microdeformation in the sense of Mindlin (1964), who considered the material element as a cell able to deform independently of the rest of the body. In such micromorphic theory (Eringen and Suhubi, 1964) the overall deformation is composed by the macroscopic continuous deformation and the internal microscopic deformation of the inner structure. This is the most successful top-down formulation of a two-level continuum model (Forest, 2013) It should be noted that the macroscopic and microscopic balance laws are postulated separately (Mindlin, 1964; Eringen and Suhubi, 1964). This poses a problem with suitable boundary conditions at the microscopic level.

One more possibility provides the introduction of internal variables to characterize the influence of a microstructure on the global behavior of a material (Coleman and Gurtin, 1967; Rice, 1971; Maugin and Muschik, 1994a). However, only the extension of the formalism of internal variables (Ván et al., 2008) ensures thermodynamically consistent hyperbolic evolution equations of internal variables (Engelbrecht and Berezovski, 2013, 2015). This extension is based on ideas of Gérard Maugin (Maugin, 1990; Maugin and Muschik, 1994a;

Maugin, 2006). In what follows, these ideas are presented systematically and results are compared with strain gradient models.

2. Historical remarks

A long history of the concept of internal variables is described in (Maugin, 2015). We point out here only basic steps. In the opinion of Truesdell (1984), Duhem was the first who introduced what are now called internal state variables. A large scale thermodynamic parameter of state was proposed by Bridgman (1943) in 1940s. Meixner and Reik (1959) introduced internal variables in the context of solid mechanics. Coleman and Gurtin (1967) presented the thermodynamic theory of *internal variables of state* with presupposed first-order evolution equations for the internal variables and without inclusion of their gradients. The internal variable theory was well formalized in 1970s (Kratochvil and Dillon Jr, 1969; Kestin and Rice, 1970; Rice, 1971; Valanis, 1972; Lubliner, 1973). The introduction of the local accompanying state concept (Bataille and Kestin, 1979; Germain et al., 1983; Bampi and Morro, 1984; Müller, 1985) enlarges the interest to internal variables. This concept was elaborated by Muschik (1990); Maugin (1990); Muschik (1991, 1993) and Kestin (1992, 1993) in 1990s. The clear distinction between internal variables of state and dynamic degrees of freedom was emphasized by Maugin and Muschik (1994a,b) in their seminal review. The general single internal variable theory enriched by the extra entropy flux is presented recently by Maugin (2006). Contemporary view on the internal variable theory can be found in (Müller and Weiss, 2012; Voyiadjis and Faghihi, 2014; Maugin, 2015).

The contribution of Professor Maugin to the advancement of the theory of internal variables cannot be overestimated. He proposed the efficient selection of the extra entropy flux (the concept introduced by Müller (1967)) in order to eliminate divergence term in the dissipation inequality (Maugin, 1990). The exposition of the theory of internal variables in (Maugin and Muschik, 1994a,b) and in (Maugin, 1999) were real landmarks for researchers. He finalized the weakly nonlocal thermomechanical theory with single internal variable in (Maugin, 2006).

3. Thermomechanical single internal variable theory

The internal variable theory supposes the extension of the state space by means of an internal variable (and its gradient of the internal variable in a weakly nonlocal theory). The internal variable φ is considered here as a second-order tensor. Then the free energy per unit volume W is specified as a sufficiently regular function of the deformation gradient $\mathbf{F}$, temperature θ, and internal variable and its gradient

$$W = \overline{W}(\mathbf{F}, \theta, \varphi, \nabla_R \varphi), \qquad (1)$$

where ∇_R denotes the gradient operator in the reference configuration.

Accordingly, the first Piola-Kirchhoff stress tensor $\mathbf{T}$, the entropy S, and affinities $\mathbf{A}$ and $\mathcal{A}$ are introduced by equations of state

$$\mathbf{T} = \frac{\partial \overline{W}}{\partial \mathbf{F}}, \quad S = -\frac{\partial \overline{W}}{\partial \theta},$$
$$\mathbf{A} = -\frac{\partial \overline{W}}{\partial \varphi}, \quad \mathcal{A} = -\frac{\partial \overline{W}}{\partial \nabla_R \varphi}. \qquad (2)$$

Following Maugin (2006), we represent the canonical balance equations of momentum and energy in the absence of body forces in the form

$$\frac{\partial \mathbf{P}}{\partial t}\bigg|_{\mathbf{X}} - Div_R \widetilde{\mathbf{b}} = \mathbf{f}^{th} + \widetilde{\mathbf{f}}^{intr}, \qquad (3)$$

$$\frac{\partial (S\theta)}{\partial t}\bigg|_{\mathbf{X}} + \nabla_R \cdot \widetilde{\mathbf{Q}} = h^{th} + \widetilde{h}^{intr}, \qquad (4)$$

with the material momentum

$$\mathbf{P} = -\rho_0 \mathbf{v} \mathbf{F}, \qquad (5)$$

the modified Eshelby stress tensor

$$\widetilde{\mathbf{b}} = -(L\mathbf{1}_R + \mathbf{T}\mathbf{F} - \mathcal{A} : (\nabla_R \varphi)^T), \qquad (6)$$

thermal sources

$$\mathbf{f}^{th} = S\nabla_R \theta, \quad h^{th} = S\dot{\theta}, \qquad (7)$$

and intrinsic source terms

$$\widetilde{\mathbf{f}}^{intr} := \widetilde{\mathcal{A}} : (\nabla_R \varphi)^T, \quad \widetilde{h}^{intr} := \widetilde{\mathcal{A}} : \dot{\varphi}. \qquad (8)$$

Here, as in (Maugin, 2006), ρ_0 is the matter density (in the reference configuration), $\mathbf{v}$ is the physical velocity, Div_R denotes the divergence operator in the reference configuration,

$$\widetilde{\mathcal{A}} = \mathbf{A} - Div_R \mathcal{A}, \quad L = K - W, \qquad (9)$$

and K is the kinetic energy per unit volume.

The balance equations are complemented by second law of thermodynamics

$$\left.\frac{\partial S}{\partial t}\right|_{\mathbf{X}} + \nabla_R \cdot \mathbf{S} \geq 0, \quad \mathbf{S} = (\mathbf{Q}/\theta) + \mathbf{K}, \quad (10)$$

which can be presented in the form of the dissipation inequality

$$(\mathbf{A} - (Div_R\mathcal{A})) : \dot{\boldsymbol{\varphi}} - \mathbf{S} \cdot \nabla_R\theta \geq 0, \quad (11)$$

if the extra entropy flux $\mathbf{K}$ is selected as (Maugin, 1990)

$$\mathbf{K} = -\theta^{-1}\mathcal{A} : \dot{\boldsymbol{\varphi}}. \quad (12)$$

3.2. Simple evolution equation for internal variable

It is clear that in the isothermal case dissipation inequality (11) is reduced to

$$\widetilde{h}^{intr} := \widetilde{\mathcal{A}} : \dot{\boldsymbol{\varphi}} \geq 0. \quad (13)$$

The simplest choice for the evolution equation for the internal variable $\boldsymbol{\varphi}$ providing the satisfaction of inequality (13) is the following:

$$\dot{\boldsymbol{\varphi}} = \mathbf{L}\widetilde{\mathcal{A}}, \quad (14)$$

with the appropriate tensor $\mathbf{L}$. The dissipation inequality will be satisfied with positive definiteness of $\mathbf{L}$

$$\widetilde{h}^{intr} = \widetilde{\mathcal{A}} : (\mathbf{L}\widetilde{\mathcal{A}}) \geq 0. \quad (15)$$

It is remarkable that evolution equation (14) takes the typical Ginzburg-Landau (or Allen-Cahn) form

$$\dot{\boldsymbol{\varphi}} = -\mathbf{L}\left(\frac{\partial \overline{W}}{\partial \boldsymbol{\varphi}} - Div_R\frac{\partial \overline{W}}{\partial (\nabla_R\boldsymbol{\varphi})}\right). \quad (16)$$

Such type of an evolution equation is commonly used in the phase field theory (Giorgi, 2009, e.g.). It can be generalized to the Cahn-Hilliard-type as well (Giorgi, 2009).

4. Strain gradient model in one dimension

Now we consider a simple one-dimensional example. The quadratic free energy function in one dimensional setting is

$$\overline{W} = \frac{\rho c^2}{2}u_x^2 + A\varphi_x u_x + \frac{1}{2}B\varphi^2 + \frac{1}{2}C\varphi_x^2, \quad (17)$$

where ρ is the density, c is the elastic wave speed in the medium without microstructure, and constant parameters A, B, and C depend on the material.

The corresponding stresses are calculated as follows:

$$\sigma = \frac{\partial \overline{W}}{\partial u_x} = \rho c^2 u_x + A\varphi_x, \quad (18)$$

$$\eta = -\frac{\partial \overline{W}}{\partial \varphi_x} = -Au_x - C\varphi_x, \quad (19)$$

and the interactive internal force τ is, respectively,

$$\tau = -\frac{\partial \overline{W}}{\partial \varphi} = -B\varphi. \quad (20)$$

The balance of linear momentum takes the form

$$\rho u_{tt} = \rho c^2 u_{xx} + A\varphi_{xx}, \quad (21)$$

and the evolution equation for the internal variable in the fully non-dissipative case (with $\widetilde{\mathcal{A}} = 0$) reduces to

$$\tau - \eta_x = C\varphi_{xx} + Au_{xx} - B\varphi = 0. \quad (22)$$

By means of Eq. (21) the latter relation can be represented in the form

$$\varphi = \frac{C}{B}\left(\rho u_{tt} - \rho c^2 u_{xx}\right) + \frac{A}{B}u_{xx}. \quad (23)$$

If coefficient C vanishes then we arrive at the strain gradient model

$$\varphi = \frac{A}{B}u_{xx}, \quad (24)$$

which results in the equation of motion of the form

$$\rho u_{tt} = \rho c^2 u_{xx} + \frac{A^2}{B}u_{xxxx}. \quad (25)$$

It should be noted that in the terms of stresses the first-order strain gradient model (24) coincides with the second-order strain gradient model in the spirit of Aifantis (Askes and Aifantis, 2011), since, following (18) and (24),

$$\sigma = \rho c^2 u_x + \frac{A^2}{B}u_{xxx}. \quad (26)$$

Accordingly, in the case of a non-zero value of the coefficient C the more general model is obtained (Berezovski et al., 2011a)

$$u_{tt} = c^2 u_{xx} + \frac{C}{B}\left(u_{tt} - c^2 u_{xx}\right)_{xx} + \frac{A^2}{\rho B}u_{xxxx}. \quad (27)$$

Thus, the strain gradient model is a restricted case in the single internal variable theory.

5. Dual internal variables

As we have seen, the single internal variable theory does not include microinertia. This theory is applicable to dissipative processes only (Maugin, 2006). The generalisation of the internal variable theory (Ván et al., 2008) unifies internal variables of state and dynamic degrees of freedom. The extension uses the theory with a single internal variable as the pattern.

Introducing two internal variables $\boldsymbol{\varphi}$ and $\boldsymbol{\psi}$ we will consider them as second-order tensors like in the case of the single internal variable. The state space is enlarged correspondingly and we have for the free energy per unit volume W

$$W = \overline{W}(\mathbf{F}, \theta, \boldsymbol{\varphi}, \nabla_R\boldsymbol{\varphi}, \boldsymbol{\psi}, \nabla_R\boldsymbol{\psi}). \qquad (28)$$

Additional affinities $\mathbf{B}$ and $\mathcal{B}$ appear in equations of state in the comparison with the case of the single internal variable

$$\mathbf{T} = \frac{\partial\overline{W}}{\partial\mathbf{F}}, \quad \mathcal{A} = -\frac{\partial\overline{W}}{\partial\nabla_R\boldsymbol{\varphi}}, \quad \mathbf{A} = -\frac{\partial\overline{W}}{\partial\boldsymbol{\varphi}},$$
$$S = -\frac{\partial\overline{W}}{\partial\theta}, \quad \mathbf{B} = -\frac{\partial\overline{W}}{\partial\boldsymbol{\psi}}, \quad \mathcal{B} = -\frac{\partial\overline{W}}{\partial\nabla_R\boldsymbol{\psi}}. \qquad (29)$$

Similarly to the case of single internal variable, the canonical equations of momentum and energy keep their form (Berezovski et al., 2011b)

$$\frac{\partial\mathbf{P}}{\partial t} - Div_R\widetilde{\mathbf{b}} = \mathbf{f}^{th} + \widetilde{\mathbf{f}}^{intr}, \qquad (30)$$

$$\frac{\partial(S\theta)}{\partial t} + \nabla_R \cdot \widetilde{\mathbf{Q}} = h^{th} + \widetilde{h}^{intr}, \qquad (31)$$

with the modified Eshelby stress tensor

$$\widetilde{\mathbf{b}} = -(L\mathbf{1}_R + \mathbf{T}\mathbf{F}). -$$
$$- (.\mathcal{A} : (\nabla_R\boldsymbol{\varphi})^T) - \mathcal{B} : (\nabla_R\boldsymbol{\psi})^T), \qquad (32)$$

and intrinsic source terms

$$\widetilde{\mathbf{f}}^{intr} := \widetilde{\mathcal{A}} : \nabla_R\boldsymbol{\varphi} + \widetilde{\mathcal{B}} : \nabla_R\boldsymbol{\psi},$$
$$\widetilde{h}^{intr} := \widetilde{\mathcal{A}} : \dot{\boldsymbol{\varphi}} + \widetilde{\mathcal{B}} : \dot{\boldsymbol{\psi}}. \qquad (33)$$

As in the case of single internal variable, the following notation is used

$$\widetilde{\mathcal{A}} = \mathbf{A} - Div_R\mathcal{A}, \qquad (34)$$

$$\widetilde{\mathcal{B}} = \mathbf{B} - Div_R\mathcal{B}, \qquad (35)$$

$$\widetilde{\mathbf{S}} = \theta^{-1}\widetilde{\mathbf{Q}}, \quad \widetilde{\mathbf{Q}} = \mathbf{Q} - \mathcal{A} : \dot{\boldsymbol{\varphi}} - \mathcal{B} : \dot{\boldsymbol{\psi}}. \qquad (36)$$

5.1. Evolution equations for internal variables

Accounting for expression of the internal heat source (33), the dissipation inequality is rewritten as follows:

$$(\mathbf{A} - (Div_R\mathcal{A})) : \dot{\boldsymbol{\varphi}} + (\mathbf{B} - (Div_R\mathcal{B})) : \dot{\boldsymbol{\psi}} +$$
$$+ \nabla_R \cdot \left(\mathcal{A} : \dot{\boldsymbol{\varphi}} + \mathcal{B} : \dot{\boldsymbol{\psi}} + \theta\mathbf{K}\right) - \qquad (37)$$
$$- \widetilde{\mathbf{S}} \cdot \nabla_R\theta \geq 0.$$

We select the extra entropy flux in the form similar to that in the case of the single internal variable

$$\mathbf{K} = -\theta^{-1}\mathcal{A} : \dot{\boldsymbol{\varphi}} - \theta^{-1}\mathcal{B} : \dot{\boldsymbol{\psi}}, \qquad (38)$$

to eliminate the divergence term in the dissipation inequality. Then the resulting dissipation inequality

$$\widetilde{h}^{intr} - \widetilde{\mathbf{S}}\nabla_R\theta \geq 0, \qquad (39)$$

is simplified in the isothermal case to

$$\widetilde{h}^{intr} = \widetilde{\mathcal{A}} : \dot{\boldsymbol{\varphi}} + \widetilde{\mathcal{B}} : \dot{\boldsymbol{\psi}} \geq 0. \qquad (40)$$

The general form of a linear solution of dissipation inequality (40) can be represented as

$$\begin{pmatrix} \dot{\boldsymbol{\varphi}} \\ \dot{\boldsymbol{\psi}} \end{pmatrix} = \begin{pmatrix} \mathbf{L}^{11} & \mathbf{L}^{12} \\ \mathbf{L}^{21} & \mathbf{L}^{22} \end{pmatrix} \begin{pmatrix} \widetilde{\mathcal{A}} \\ \widetilde{\mathcal{B}} \end{pmatrix}, \qquad (41)$$

where components $\mathbf{L}^{11}, ..., \mathbf{L}^{22}$ of the linear operator $\mathbf{L}$ are dependent on state variables (Gurtin, 1996).

The specific form of the evolution equations for the internal variables $\boldsymbol{\varphi}$ and $\boldsymbol{\psi}$ depends on the values of components of the linear operator $\mathbf{L}$.

5.2. Non-dissipative case

To avoid dissipative effects, we are forced to use the skew-symmetric case ($\mathbf{L}^{11} = \mathbf{L}^{22} = \mathbf{0}$ and $\mathbf{L}^{12} = -\mathbf{L}^{21}$). In this case, evolution equations for the two internal variables are fully coupled

$$\dot{\boldsymbol{\varphi}} = \mathbf{L}^{12}\widetilde{\mathcal{B}}, \quad \dot{\boldsymbol{\psi}} = -\mathbf{L}^{12}\widetilde{\mathcal{A}}, \qquad (42)$$

and the dissipation $\widetilde{h}^{intr}$ vanishes. It should be noted that the evolution of one internal variable is driven by another one that means the duality between the internal variables.

6. Microstructure model in one dimension

As an example, let us consider one-dimensional case. Specifically, we can derive a microstructure model having the evolution equations for internal variables in the non-dissipative case. We start with a quadratic free energy dependence (Berezovski et al., 2011a)

$$\overline{W} = \frac{\rho c^2}{2} u_x^2 + A\varphi_x u_x + \frac{1}{2} B\varphi^2 + \frac{1}{2} C\varphi_x^2 + \frac{1}{2} D\psi^2, \tag{43}$$

where, as before, $A, B, C,$ and D are material parameters characterizing microstructure influence.

For simplicity, only the contribution of the second internal variable itself is included. Then we can calculate stresses

$$\sigma = \frac{\partial \overline{W}}{\partial u_x} = \rho c^2 u_x + A\varphi_x, \tag{44}$$
$$\eta = -\frac{\partial \overline{W}}{\partial \varphi_x} = -Au_x - C\varphi_x, \zeta = -\frac{\partial \overline{W}}{\partial \psi_x} = 0,$$

and the interactive internal force τ

$$\tau = -\frac{\partial \overline{W}}{\partial \varphi} = -B\varphi. \tag{45}$$

The affinity with respect to the dual internal variable is, respectively,

$$\xi = -\frac{\partial \overline{W}}{\partial \psi} = -D\psi. \tag{46}$$

In the isothermal case, the dissipation inequality reduces to the intrinsic part depending only on internal variables

$$\widetilde{h}^{intr} = (\tau - \eta_x)\varphi_t + (\xi - \zeta_x)\psi_t \geq 0. \tag{47}$$

It is easy to see that the choice

$$\varphi_t = R(\xi - \zeta_x), \qquad \psi_t = -R(\tau - \eta_x), \tag{48}$$

where R is an appropriate constant, leads to zero dissipation. Therefore, dissipation inequality (47) is satisfied automatically with choice (48). In the non-dissipative case, evolution equation for the internal variable φ (48)$_1$ can be presented as

$$\varphi_t = -RD\psi. \tag{49}$$

Making the time differentiation of Eq. (49) and taking into account the evolution equation for the

dual internal variable (48)$_2$ we arrive at the hyperbolic equation for the internal variable φ

$$\varphi_{tt} = R^2 D(\tau - \eta_x). \tag{50}$$

Now we can represent the equations of motion both for macroscale and microscale in the form, which includes the internal variable φ only

$$\rho u_{tt} = \rho c^2 u_{xx} + A\varphi_{xx}, \tag{51}$$

$$I\varphi_{tt} = C\varphi_{xx} + Au_{xx} - B\varphi, \tag{52}$$

where $I = 1/(R^2 D)$.

The constructed model describing the influence of microstructure by means of dual internal variables is non-dissipative. Equations of motion at both macro- and micro-levels are hyperbolic. The hyperbolicity of the equation of motion at the microlevel is a direct consequence of the non-dissipativity requirement.

6.1. Single dispersive wave equation

It is possible to obtain a single wave equation from Eqs. (51) and (52). To do that we determine the second space derivative of the internal variable from Eq. (52)

$$\varphi_{xx} = -\frac{I}{B}\varphi_{ttxx} + \frac{C}{B}\varphi_{xxxx} + \frac{A}{B}u_{xxxx}, \tag{53}$$

and its fourth derivatives from Eq. (51)

$$\frac{A}{\rho}\varphi_{xxxx} = \left(u_{tt} - c^2 u_{xx}\right)_{xx}, \\ \frac{A}{\rho}\varphi_{ttxx} = \left(u_{tt} - c^2 u_{xx}\right)_{tt}. \tag{54}$$

Inserting the results into balance of linear momentum (51), we obtain the fourth-order equation

$$u_{tt} = c^2 u_{xx} + \frac{C}{B}\left(u_{tt} - c^2 u_{xx}\right)_{xx} - \\ - \frac{I}{B}\left(u_{tt} - c^2 u_{xx}\right)_{tt} + \frac{A^2}{\rho B}u_{xxxx}. \tag{55}$$

This is a general dispersive wave equation for the Mindlin-type model of the microstructure influence (Berezovski et al., 2011a).

6.2. Remark on strain gradient models

Since the strain gradient has not its own inertia, the coefficient I vanishes if the internal variable φ is identified with the strain gradient. In such

5

a case, the remaining part of Eq. (55) coincides with Eq. (27) obtained in the case of a single internal variable. This means that the strain gradient models are constrained having only some limited nonlocality due to the appearance of an internal length scale. Moreover, as it is noted by Chen et al. (2003), "classical continuum theory, the gradient theories, and the couple stress theories do not stem from the considerations of microstructure or micromotion and as a consequence, would break down if the micromotion and/or the microstructure become too significant to be neglected."

7. Conclusions

The use of internal variables for the description of the influence of a microstructure on the overall behavior of solids is not new idea. However, for a long time internal variables of state have been used for the accounting of internal dissipation in contrast to dynamic degrees of freedom, which possess their own balances. The introduction of dual internal variables unifies the treatment both internal variables of state and dynamic degrees of freedom (Ván et al., 2008). Both parabolic evolution equations for dissipative internal variables and hyperbolic evolution equations in the absence of dissipation are covered by the extension of the theory of internal variables. Evolution equations for internal variables follow from the dissipation inequality and, therefore, are thermodynamically consistent. The structure of well known evolution equations for the Cosserat microrotation and for the micromorphic microdeformation is recovered in the framework of the proposed approach (Berezovski et al., 2011b; Ván et al., 2014). This approach is more flexible and powerful than less sophisticated and therefore more popular phase field and strain gradient models.

The given description of the dual internal variables is constrained by non-dissipative processes. The complete dual internal variables theory comprising thermal effects can be found in (Berezovski and Ván, 2017). It should be emphasized once more that the dual internal variables theory is a direct extension and continuation of the single internal variable theory accomplished by Maugin (2006).

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