Thermoelasticity with dual internal variables

Arkadi Berezovski[*], **Jüri Engelbrecht**

Centre for Nonlinear Studies

Institute of Cybernetics at Tallinn University of Technology

Akadeemia tee 21, 12618 Tallinn, Estonia

Gérard A. Maugin

Institut Jean Le Rond d'Alembert, Université Pierre et Marie Curie

UMR 7190, Case 162, 4 Place Jussieu, 75252, Paris Cédex 05, France

Abstract

The extension of the thermoelasticity theory by weakly non-local dual internal variables enriched by an extra entropy flux for the thermomechanical description of the behavior of microstructured solids is presented. The internal variables take into account the distributed effect of microdeformations or microtemperatures (and their gradients) on the overall macroscopic behavior. The evolution equations for microtemperatures can be hyperbolic, which can induce wave-like propagation for macrotemperature due to the coupling of equations.

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[*] Corresponding author, e-mail: Arkadi.Berezovski@cs.ioc.ee, Phone: +372 6204164, Fax: +372 6204151

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1 Motivation

Thermoelasticity is a generic multiphysics and multiscale theory because it combines mechanical and thermal phenomena, each of which has its own time scale. In (quasi)statics, the exchange of heat with the environment is complete during a slow increase of loading and the resulting deformation. A constant temperature over the entire solid is kept, called the temperature of the natural state. In contrast, in dynamics the heat exchange due to heat conduction is very slow. If there are no heat sources within the solid, then we arrive at the conditions of an adiabatic process. In the theory of thermal stresses, the effect of the change of deformation on the deviation of temperature is neglected. The equation of heat conduction is derived without taking the body deformation into account. The theory of coupled thermoelasticity unifies differential equations for all possible thermodynamic processes [1, 2].

The response of many materials of engineering interest (e.g., metals, alloys, granular materials, composites, liquid crystals, polycrystals) to external loading is often influenced by an existing or emergent microstructure (e.g., phases in multiphase materials, voids, microcracks, dislocation substructures, texture). In general, the components of such a microstructure have different material properties, resulting in a macroscopic material behavior which is highly anisotropic and inhomogeneous. Prediction of the thermoelastic behavior of such materials is not an easy task, because in addition to the generalized continuum description extending the conventional continuum mechanics for incorporating intrinsic microstructural effects in the mechanical behavior of materials [3–6], a more general description of thermal processes is also needed.

Generalized heat conduction means usually a hyperbolic heat propagation with the Cattaneo-Vernotte or Jeffreys constitutive relation for the heat flux [7–10], which reflects in generalization of thermoelasticity [9, 10] based on earlier studies by Lord and Shulman [11] and Green and Lindsay [12]. The "thermoelasticity with finite wave speed" [10] as well as the thermal displacement variable theory by Green and Naghdi [13–15] deal with the macroscopic temperature without any reference to microstructure. From another side, the combination of generalized continua theories of Eringen [6] or Green and Naghdi [13] with microtemperatures in the spirit of Grot [16] presented in the series of papers by Ieşan and his co-authors [17–19] is an exotic exercise due the difficulty in the interpretation of the microtemperature as a vector.

It is well known that in the conventional thermoelasticity the free energy density is a function of the deformation gradient and temperature only and cannot depend on the temperature gradient [20, 21]. However, in the presence of varying temperature fields at the microstructure level, temperature gradient effects on the thermomechanical response of the material are expected due to the microheterogeneous nature of materials. In order to take such effects into account a thermoelastic constitutive equation for second grade media was proposed by Cardona, Forest and Sievert [22], and the gradient of entropy model was developed [23]. However, the resulting heat conduction equation deviates from the classical heat equation only by an additional contribution which is proportional to the Laplacian of the temperature rate of change.

Internal variable approach was always an alternative framework for the continuum modeling of materials (cf. [24]). The thermodynamic theory of internal variables presented by Coleman and Gurtin [25] had presupposed first-order evolution equations for the internal variables and did not include their gradients. Accounting for the gradients leads to the weakly nonlocal theory [26, 27], which can be also enriched by the extra entropy flux [28]. The complete theory of the internal state variables is presented recently by Maugin [29, 30]. Moreover, the limitation of evolution equations by only first-order ones is got over by the concept of dual internal variables [31]. As it was demonstrated [32–34], this concept allows to recover the structure of Cosserat, micromorphic, and second gradient elasticity theories in a natural way. It should be noted, however, that the mentioned results are obtained in the isothermal setting. However, temperature can be also treated as an internal variable (cf. [35]).

In this paper, the desired extension of the dual internal variable approach to the thermoelastic description of microstructured solids is presented. It appears that in the framework of the internal variables theory it is possible to obtain a hyperbolic evolution equation for microtemperatures keeping the parabolic evolution equation for the macrotemperature. Effects of microtemperature gradients exhibit themselves on the macrolevel due to the coupling of equations of macromotion and evolution equations for macro- and microtemperatures.

The most suitable framework for the generalization of continuum theory by weakly non-local dual internal variables enriched by an extra entropy flux is the material formulation of thermomechanics [36]. Therefore, basic definitions of canonical thermomechanics [36] are recalled in the next section of the paper. This is followed by the reminder of the conventional theory of single internal variable of state [29, 30]. Then dual variables are introduced and evolution equations for them are derived. The comparison with the GENERIC approach [37] shows that the dual internal variables can provide a contribution in both reversible and dissipative processes in a microstructured medium. As an example, the one-dimensional thermoelasticity theory is considered in detail.

2 Canonical thermomechanics

The starting point for the representation of the dual internal variable theory is the canonical thermomechanics or the thermomechanics in material formulation [36]. Considering the motion of a body as a time-parametrized mapping χ connecting a material point $\mathbf{X}$ with Cartesian coordinates (X_1, X_2, X_3) in the reference configuration and its position $\mathbf{x}$ with Cartesian coordinates (x_1, x_2, x_3) in the actual configuration in Euclidean physical space,

$$\mathbf{x} = \chi(\mathbf{X}, t), \quad \text{or} \quad x_i = \chi(X_k, t), \quad i, k = 1, 2, 3, \tag{1}$$

we can write the local balance laws in so-called Piola-Kirchhoff formulation 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 (cf. Maugin [36]) as the mass conservation

$$\left.\frac{\partial \rho_0}{\partial t}\right|_{\mathbf{X}} = 0, \tag{2}$$

the balance of linear momentum

$$\left.\frac{\partial (\rho_0 \mathbf{v})}{\partial t}\right|_{\mathbf{X}} - Div_R \mathbf{T} = \mathbf{f}_0, \tag{3}$$

and the energy conservation equation

$$\left.\frac{\partial (K + E)}{\partial t}\right|_{\mathbf{X}} - \nabla_R \cdot (\mathbf{T} \cdot \mathbf{v} - \mathbf{Q}) = \mathbf{f}_0 \cdot \mathbf{v}. \tag{4}$$

The balance laws (2)-(4) are complemented by the second law of thermodynamics

$$\left.\frac{\partial S}{\partial t}\right|_{\mathbf{X}} + \nabla_R \cdot \mathbf{S} \geq 0, \quad \mathbf{S} = (\mathbf{Q}/\theta) + \mathbf{J}. \tag{5}$$

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. Accordingly, the deformation gradient is defined by

$$\mathbf{F} = \left.\frac{\partial \chi}{\partial \mathbf{X}}\right|_t = \nabla_R \chi. \tag{6}$$

The so-called theorem of the kinetic energy is obtained be multiplying Eq. (3) by $\mathbf{v}$:

$$\left.\frac{\partial K}{\partial t}\right|_{\mathbf{X}} - \nabla_R \cdot (\mathbf{T} \cdot \mathbf{v}) + \mathbf{T} : \dot{\mathbf{F}} - \mathbf{f}_0 \cdot \mathbf{v} = 0. \tag{7}$$

The combination of the theorem of kinetic energy (7) with the energy conservation (4) results in the so-called theorem of internal energy:

$$\left.\frac{\partial E}{\partial t}\right|_{\mathbf{X}} - \mathbf{T} : \dot{\mathbf{F}} + \nabla_R \cdot \mathbf{Q} = 0. \tag{8}$$

Introducing the Helmholtz free energy function by $W = E - \theta S$, we can rewrite Eq. (8) in the canonical form of the energy conservation for sufficiently smooth fields at any regular material point $\mathbf{X}$ in the body [29, 30]

$$\left.\frac{\partial (S\theta)}{\partial t}\right|_{\mathbf{X}} + \nabla_R \cdot \mathbf{Q} = h^{int}, \quad h^{int} := \mathbf{T} : \dot{\mathbf{F}} - \left.\frac{\partial W}{\partial t}\right|_{\mathbf{X}}. \tag{9}$$

The right-hand side of Eq. $(9)_1$ is formally an internal heat source.

Correspondingly, the canonical (material) momentum balance equation in the presence of a body force $\mathbf{f}_0$ per unit reference volume can be obtained by multiplying the balance of linear momentum (3) by the deformation gradient [29, 30]. The result is

$$\left.\frac{\partial \mathbf{P}}{\partial t}\right|_{\mathbf{X}} - Div_R \mathbf{b} = \mathbf{f}^{int} + \mathbf{f}^{ext} + \mathbf{f}^{inh}, \tag{10}$$

where the *material momentum* **P**, the material *Eshelby stress* **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

$$\mathbf{P} := -\rho_0 \mathbf{v} \cdot \mathbf{F}, \quad \mathbf{b} = -\left(L\mathbf{I}_R + \mathbf{T}.\mathbf{F}\right), \quad L = K - W, \tag{11}$$

$$\mathbf{f}^{inh} := \left.\frac{\partial L}{\partial \mathbf{X}}\right|_{expl} \equiv \left.\frac{\partial L}{\partial \mathbf{X}}\right|_{fixed\ fields} = \left(\frac{1}{2}\mathbf{v}^2\right) \nabla_R \rho_0 - \left.\frac{\partial W}{\partial \mathbf{X}}\right|_{expl}, \tag{12}$$

$$\mathbf{f}^{ext} := -\mathbf{f}_0 \cdot \mathbf{F}, \quad \mathbf{f}^{int} = \mathbf{T} : (\nabla_R \mathbf{F})^T - \left.\nabla_R W\right|_{impl}. \tag{13}$$

Here the subscript notations *expl* and *impl* mean, respectively, the material gradient keeping the fields fixed (and thus extracting the explicit dependence on **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 (5) multiplied by θ yields the celebrated Clausius-Duhem inequality

$$-\left.\left(\frac{\partial W}{\partial t} + S\frac{\partial \theta}{\partial t}\right)\right|_{\mathbf{X}} + \mathbf{T} : \dot{\mathbf{F}} + \nabla_R \cdot (\theta \mathbf{J}) - \mathbf{S} \cdot \nabla_R \theta \geq 0. \tag{14}$$

Now we are equipped for the introduction of internal variables. It may be instructive to remind first the theory with a single internal variable recently presented in a comprehensive form by Maugin [29, 30].

3 Single internal variable

Up to now the microstructure was not specified. It can be prescribed by the specification of location, shape, and properties of inclusions, as, for example, in the case of periodic structures. If the microstructure is irregular, such a prescription is impossible. In the framework of the phenomenological continuum theory it is assumed that the influence of the microstructure on the overall macroscopic behavior can be taken into account by the introduction of an internal variable φ which we associate with the distributed effect of the microstructure.

Formally, the introduction of an internal variable means that the state space of a material point is described not only by the deformation gradient and temperature, but also by the internal variable and its gradient. Usually, the introduction of an internal variable is made without the specification of its tensorial nature. To be more precise, we will consider the internal variable of state $\boldsymbol{\alpha}$ as a second-order tensor. Then the free energy per unit volume W is specified as the general sufficiently regular function

$$W = \overline{W}(\mathbf{F}, \theta, \boldsymbol{\alpha}, \nabla_R \boldsymbol{\alpha}). \tag{15}$$

The corresponding equations of state are given by [29, 30]

$$\mathbf{T} = \frac{\partial \overline{W}}{\partial \mathbf{F}}, \quad S = -\frac{\partial \overline{W}}{\partial \theta}, \quad \mathbf{A} := -\frac{\partial \overline{W}}{\partial \boldsymbol{\alpha}}, \quad \mathscr{A} := -\frac{\partial \overline{W}}{\partial \nabla_R \boldsymbol{\alpha}}. \tag{16}$$

The presence of internal variables leads to a modification of the governing balance laws. To be consistent, let us consider first the dissipation inequality (14), which is represented as

$$\Phi = (\mathbf{A} - Div_R \mathscr{A}) : \dot{\boldsymbol{\alpha}} + \nabla_R \cdot (\mathscr{A} : \dot{\boldsymbol{\alpha}} + \theta \mathbf{K}) - \mathbf{S} \cdot \nabla_R \theta \geq 0. \tag{17}$$

Following Maugin [28], we select the extra entropy flux in order to eliminate the divergence term in Eq. (17)

$$\mathbf{J} = -\theta^{-1} \mathscr{A} : \dot{\boldsymbol{\alpha}}. \tag{18}$$

Such a choice results in the canonical equations of momentum and energy in the form [29, 30]

$$\left.\frac{\partial \mathbf{P}}{\partial t}\right|_{\mathbf{X}} - Div_R \widetilde{\mathbf{b}} = \mathbf{f}^{th} + \widetilde{\mathbf{f}}^{intr}, \tag{19}$$

$$\left.\frac{\partial (S\theta)}{\partial t}\right|_{\mathbf{X}} + \nabla_R \cdot \widetilde{\mathbf{Q}} = h^{th} + \widetilde{h}^{intr}. \tag{20}$$

Here the introduced thermal source terms involve only temperature

$$\mathbf{f}^{th} = S\nabla_R \theta, \quad h^{th} = S\dot{\theta}, \tag{21}$$

whereas "intrinsic" source terms are determined by the internal variable

$$\widetilde{\mathbf{f}}^{intr} := \widetilde{\mathscr{A}} : (\nabla_R \boldsymbol{\alpha})^T, \quad \widetilde{h}^{intr} := \widetilde{\mathscr{A}} : \dot{\boldsymbol{\alpha}}. \tag{22}$$

The modified Eshelby stress tensor

$$\widetilde{\mathbf{b}} = -(L\mathbf{I}_R + \mathbf{T}.\mathbf{F} - \mathscr{A} : (\nabla_R \boldsymbol{\alpha})^T), \tag{23}$$

includes all effects presenting gradients since the material gradient of $\boldsymbol{\alpha}$ plays a role parallel to that of the deformation gradient $\mathbf{F}$. Remaining modifications are defined as follows [29, 30]

$$\widetilde{\mathscr{A}} \equiv -\delta_{\boldsymbol{\alpha}} \overline{W} := -\left(\frac{\partial \overline{W}}{\partial \boldsymbol{\alpha}} - Div_R \frac{\partial \overline{W}}{\partial (\nabla_R \boldsymbol{\alpha})}\right) = \mathbf{A} - Div_R \mathscr{A}, \tag{24}$$

$$\widetilde{\mathbf{S}} = \theta^{-1} \widetilde{\mathbf{Q}}, \quad \widetilde{\mathbf{Q}} = \mathbf{Q} - \mathscr{A} : \dot{\boldsymbol{\alpha}}, \tag{25}$$

and the dissipation inequality is represented as

$$\Phi = \widetilde{\mathscr{A}} : \dot{\boldsymbol{\alpha}} - \widetilde{\mathbf{S}} \nabla_R \theta \geq 0. \tag{26}$$

The main advantage of the use of the material formulation of thermomechanics is the conservation of the form of the canonical balance laws and clear separation of thermal and intrinsic dissipation. If we assume that intrinsic dissipation is still independent of temperature gradient, then we are forced to modify the Fourier's law

$$\mathbf{Q} - \mathscr{A} : \dot{\boldsymbol{\alpha}} = -a^2 \nabla_R \theta. \tag{27}$$

The standard choice to provide the non-negativity of the intrinsic part of the dissipation inequality (26)

$$\widetilde{h}^{intr} = \widetilde{\mathscr{A}} : \dot{\boldsymbol{\alpha}} \geq 0, \tag{28}$$

leads to the evolution equation for the internal variable in the form

$$\dot{\boldsymbol{\alpha}} = k\widetilde{\mathscr{A}}, \quad k \geq 0. \tag{29}$$

The obtained reaction-diffusion-like equation

$$\dot{\boldsymbol{\alpha}} = k(\mathbf{A} - Div_R \mathscr{A}), \tag{30}$$

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

$$W = \overline{W}(..., \alpha, \nabla_R \alpha) = f(..., \alpha) + \frac{1}{2} D (\nabla \alpha)^2, \tag{31}$$

we arrive at the Ginzburg-Landau (or the Allen-Cahn) equation (cf. Cross and Hohenberg [38])

$$\frac{1}{k} \dot{\alpha} = D \nabla^2 \alpha - f'(\alpha), \tag{32}$$

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

If we identify the internal variable with microtemperature, then we can see that its evolution is described by a parabolic equation similarly to the macroscopic heat conduction equation. The influence of a microstructure is exhibited only by the distinction in heat conduction coefficients at macro- and microlevels.

A more general description of the thermoelastic behavior of microstructured solids can be provided by the dual internal variable approach [31], as demonstrated in the isothermal situation [32–34]. The introduction of an additional internal variable extends not only the state space, but also the structure of the corresponding theory.

4 Dual internal variables

The generalization of the internal variable theory to the case of two internal variables is straightforward [34]. Let us consider the free energy W as a function of two internal variables, $\boldsymbol{\alpha}$ and $\boldsymbol{\beta}$, each of which is a second-order tensor

$$W = \overline{W}(\mathbf{F}, \theta, \boldsymbol{\alpha}, \nabla_R \boldsymbol{\alpha}, \boldsymbol{\beta}, \nabla_R \boldsymbol{\beta}). \tag{33}$$

In this case, the equations of state are given by

$$\begin{gathered}\mathbf{T} = \frac{\partial \overline{W}}{\partial \mathbf{F}}, \quad S = -\frac{\partial \overline{W}}{\partial \theta}, \quad \mathbf{A} := -\frac{\partial \overline{W}}{\partial \boldsymbol{\alpha}}, \quad \mathscr{A} := -\frac{\partial \overline{W}}{\partial \nabla_R \boldsymbol{\alpha}}, \\ \mathbf{B} := -\frac{\partial \overline{W}}{\partial \boldsymbol{\beta}}, \quad \mathscr{B} := -\frac{\partial \overline{W}}{\partial \nabla_R \boldsymbol{\beta}}.\end{gathered} \tag{34}$$

We include into consideration the non-zero extra entropy flux according to the case of the single internal variable

$$\mathbf{J} = -\theta^{-1} \mathscr{A} : \dot{\boldsymbol{\alpha}} - \theta^{-1} \mathscr{B} : \dot{\boldsymbol{\beta}}. \tag{35}$$

The canonical equations of momentum and energy keep their form

$$\begin{aligned}\left.\frac{\partial \mathbf{P}}{\partial t}\right|_{\mathbf{X}} - Div_R \widetilde{\mathbf{b}} &= \mathbf{f}^{th} + \widetilde{\mathbf{f}}^{intr}, \\ \left.\frac{\partial (S\theta)}{\partial t}\right|_{\mathbf{X}} + \nabla_R \cdot \widetilde{\mathbf{Q}} &= h^{th} + \widetilde{h}^{intr},\end{aligned} \tag{36}$$

with the modified Eshelby stress tensor

$$\widetilde{\mathbf{b}} = -(L \mathbf{1}_R + \mathbf{T}.\mathbf{F} - \mathscr{A} : (\nabla_R \boldsymbol{\alpha})^T - \mathscr{B} : (\nabla_R \boldsymbol{\beta})^T), \tag{37}$$

and intrinsic source terms

$$\widetilde{\mathbf{f}}^{intr} := \widetilde{\mathscr{A}} : \nabla_R \boldsymbol{\alpha} + \widetilde{\mathscr{B}} : \nabla_R \boldsymbol{\beta}, \quad \widetilde{h}^{intr} := \widetilde{\mathscr{A}} : \dot{\boldsymbol{\alpha}} + \widetilde{\mathscr{B}} : \dot{\boldsymbol{\beta}}. \tag{38}$$

In the above equations the following definitions are used

$$\widetilde{\mathscr{A}} \equiv -\delta_{\boldsymbol{\alpha}} \overline{W} := -\left(\frac{\partial \overline{W}}{\partial \boldsymbol{\alpha}} - Div_R \frac{\partial \overline{W}}{\partial (\nabla_R \boldsymbol{\alpha})} \right) = \mathbf{A} - Div_R \mathscr{A}, \tag{39}$$

$$\widetilde{\mathscr{B}} \equiv -\delta_{\boldsymbol{\beta}} \overline{W} := -\left(\frac{\partial \overline{W}}{\partial \boldsymbol{\beta}} - Div_R \frac{\partial \overline{W}}{\partial (\nabla_R \boldsymbol{\beta})} \right) = \mathbf{B} - Div_R \mathscr{B}, \tag{40}$$

$$\widetilde{\mathbf{S}} = \theta^{-1} \widetilde{\mathbf{Q}}, \quad \widetilde{\mathbf{Q}} = \mathbf{Q} - \mathscr{A} : \dot{\boldsymbol{\alpha}} - \mathscr{B} : \dot{\boldsymbol{\beta}}, \tag{41}$$

which are similar to those in the case of the single internal variable.

The corresponding dissipation inequality

$$\Phi = \widetilde{\mathscr{A}} : \dot{\boldsymbol{\alpha}} + \widetilde{\mathscr{B}} : \dot{\boldsymbol{\beta}} - \widetilde{\mathbf{S}} \nabla_R \theta \geq 0, \tag{42}$$

again contains both intrinsic and thermal parts. The thermal part of this inequality can be satisfied by the modification of Fourier's law

$$\mathbf{Q} - \mathscr{A} : \dot{\boldsymbol{\alpha}} - \mathscr{B} : \dot{\boldsymbol{\beta}} = -a^2 \nabla_R \theta. \tag{43}$$

The intrinsic part of the dissipation inequality (42) has the form

$$\widetilde{h}^{intr} := \widetilde{\mathscr{A}} : \dot{\boldsymbol{\alpha}} + \widetilde{\mathscr{B}} : \dot{\boldsymbol{\beta}} \geq 0. \tag{44}$$

The introduction of the second internal variable results in a more general form of evolution equations for the internal variables $\boldsymbol{\alpha}$ and $\boldsymbol{\beta}$, which in accordance with Eq. (44) are chosen as

$$\begin{pmatrix} \dot{\boldsymbol{\alpha}} \\ \dot{\boldsymbol{\beta}} \end{pmatrix} = \mathbf{R} \begin{pmatrix} \widetilde{\mathscr{A}} \\ \widetilde{\mathscr{B}} \end{pmatrix}, \quad \text{or} \quad \begin{pmatrix} \dot{\boldsymbol{\alpha}} \\ \dot{\boldsymbol{\beta}} \end{pmatrix} = \begin{pmatrix} \mathbf{R}^{11} & \mathbf{R}^{12} \\ \mathbf{R}^{21} & \mathbf{R}^{22} \end{pmatrix} \begin{pmatrix} \widetilde{\mathscr{A}} \\ \widetilde{\mathscr{B}} \end{pmatrix}, \tag{45}$$

where components $\mathbf{R}^{11}, ..., \mathbf{R}^{22}$ of the linear operator $\mathbf{R}$ are dependent on state variables [39].

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.

$$\begin{aligned}\begin{pmatrix}\dot{\boldsymbol{\alpha}}\\ \dot{\boldsymbol{\beta}}\end{pmatrix} = &\begin{pmatrix}\mathbf{R}^{11} & (\mathbf{R}^{12}+\mathbf{R}^{21})/2\\ (\mathbf{R}^{21}+\mathbf{R}^{12})/2 & \mathbf{R}^{22}\end{pmatrix}\begin{pmatrix}\widetilde{\mathscr{A}}\\ \widetilde{\mathscr{B}}\end{pmatrix} +\\ &+\begin{pmatrix}0 & (\mathbf{R}^{12}-\mathbf{R}^{21})/2\\ (\mathbf{R}^{21}-\mathbf{R}^{12})/2 & 0\end{pmatrix}\begin{pmatrix}\widetilde{\mathscr{A}}\\ \widetilde{\mathscr{B}}\end{pmatrix},\end{aligned} \tag{46}$$

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 anti-symmetric 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. However, we have no reasons to assume the symmetry of the linear operator $\mathbf{R}$ in the case of arbitrary internal variables.

In the case of linear elasticity without body forces, we can represent the equations of motion and energy in the form of a dissipative Hamiltonian system (cf. Mielke [40]) introducing the displacement vector $\mathbf{u}$ and momentum $p = \rho_0\dot{\mathbf{u}}$

$$\begin{pmatrix}\dot{\mathbf{u}}\\ \dot{\mathbf{p}}\\ \dot{\boldsymbol{\alpha}}\\ \dot{\boldsymbol{\beta}}\\ \dot{\theta}\end{pmatrix} = \begin{pmatrix}0 & 1 & 0 & 0 & 0\\ -1 & 0 & 0 & 0 & 0\\ 0 & 0 & -\mathbf{R}^{11} & -\mathbf{R}^{12} & 0\\ 0 & 0 & -\mathbf{R}^{21} & -\mathbf{R}^{22} & 0\\ 0 & 0 & 0 & 0 & -\frac{\boldsymbol{\Lambda}}{\theta_0}\end{pmatrix}\begin{pmatrix}\delta_{\mathbf{p}}H\\ \delta_{\mathbf{u}}H\\ \delta_{\boldsymbol{\alpha}}H\\ \delta_{\boldsymbol{\beta}}H\\ \delta_{\theta}H\end{pmatrix} + \begin{pmatrix}0\\ 0\\ 0\\ 0\\ F(\theta-\theta_0)+\widetilde{h}^{intr}\end{pmatrix}, \tag{47}$$

where variational derivatives of the "Hamiltonian" $H = E - \theta S = K + U - \theta S = K + W$ are defined as

$$\delta_{\mathbf{w}}H = \partial_{\mathbf{w}}H - Div_R\left(\partial_{\nabla\mathbf{w}}H\right), \quad \delta_{\theta}H = \partial_{\theta}H, \tag{48}$$

$\boldsymbol{\Lambda}$ is a heat conduction operator, F is a coupling operator, $\mathbf{w}$ denotes state variables $\mathbf{u}, \mathbf{p}, \boldsymbol{\alpha}, \boldsymbol{\beta}$, and θ_0 is the reference temperature and only small deviations from it are considered.

If we decompose the matrix of the system of Eqs. (47) into symmetric and antisymmetric parts

$$\begin{pmatrix} 0 & 1 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & \mathbf{R}^{11} & \mathbf{R}^{12} & 0 \\ 0 & 0 & \mathbf{R}^{21} & \mathbf{R}^{22} & 0 \\ 0 & 0 & 0 & 0 & -\frac{\mathbf{\Lambda}}{\theta_0} \end{pmatrix} = L - N = \tag{49}$$

$$= \begin{pmatrix} 0 & 1 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\mathbf{R}^{12}-\mathbf{R}^{21}}{2} & 0 \\ 0 & 0 & -\frac{\mathbf{R}^{21}-\mathbf{R}^{12}}{2} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix} - \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \mathbf{R}^{11} & \frac{\mathbf{R}^{12}+\mathbf{R}^{21}}{2} & 0 \\ 0 & 0 & \frac{\mathbf{R}^{21}+\mathbf{R}^{12}}{2} & \mathbf{R}^{22} & 0 \\ 0 & 0 & 0 & 0 & \frac{\mathbf{\Lambda}}{\theta_0} \end{pmatrix},$$

then we can see that the system of equations (47) has a metriplectic structure [40]

$$\dot{Z} = (L(Z) - N(Z))\delta H(Z) + F(Z), \tag{50}$$

where $Z = (\mathbf{w}, \theta)$, the antisymmetric part L corresponds to a Poisson structure, and the symmetric and positive semidefinite part N defines a dissipation structure.

As shown by Mielke [40], the metriplectic formulation (50) is a reduced form of the GENERIC formulation [37]

$$\dot{Z} = L(Z)D\mathscr{E}(Z) + M(Z)D\mathscr{S}(Z) + F(Z), \tag{51}$$

with the energy functional $\mathscr{E}$ and the entropy functional $\mathscr{S}$ given as follows [40]:

$$\begin{aligned}
&\mathscr{E}(\mathbf{u},\mathbf{p},\boldsymbol{\alpha},\boldsymbol{\beta},\theta) = \\
&\int_\Omega E(X,\mathbf{u}(X),\nabla\mathbf{u}(X),\mathbf{p}(X),\boldsymbol{\alpha}(X),\nabla\boldsymbol{\alpha}(X),\boldsymbol{\beta}(X),\nabla\boldsymbol{\beta}(X),\theta(X))dX, \\
&\text{with}\quad E(X,\mathbf{u},\nabla\mathbf{u},\mathbf{p},\boldsymbol{\alpha},\nabla\boldsymbol{\alpha},\boldsymbol{\beta},\nabla\boldsymbol{\beta},\theta) = \frac{\mathbf{p}^2}{2\rho_0} + U(X,\nabla\mathbf{u},\boldsymbol{\alpha},\nabla\boldsymbol{\alpha},\boldsymbol{\beta},\nabla\boldsymbol{\beta},\theta), \\
&\mathscr{S}(\mathbf{u},\boldsymbol{\alpha},\boldsymbol{\beta},\theta) = \int_\Omega S(X,\nabla\mathbf{u}(X),\boldsymbol{\alpha}(X),\nabla\boldsymbol{\alpha}(X),\boldsymbol{\beta}(X),\nabla\boldsymbol{\beta}(X),\theta(X))dX,
\end{aligned} \tag{52}$$

and

$$\mathscr{H} = \mathscr{E} - \theta_0\mathscr{S}, \quad \mathscr{H}(w,\nabla w,\theta) = \int_\Omega H(w(X),\nabla w(X),\theta(X))dX, \tag{53}$$

$$D_w\mathscr{H} = \delta_w H, \quad D_\theta\mathscr{H} = \delta_\theta H, \quad N = -\frac{1}{\theta_0}M. \tag{54}$$

As one can see, the contribution of internal variables into the reversible Poisson structure is possible only in the case of dual internal variables, whereas a single internal variable is involved exclusively in the dissipation structure.

In order to demonstrate how particular forms of evolution equations for internal variables can be derived we consider the example of one-dimensional thermoelasticity.

5 One-dimensional thermoelasticity in solids with microstructure

The one-dimensional motion of the thermoelastic conductors of heat is governed by local balance laws for linear momentum and energy (no body forces)

$$(\rho_0 v)_t - \sigma_x = 0, \tag{55}$$

$$\left(\frac{1}{2}\rho_0 v^2 + E\right)_t - (\sigma v - Q)_x = 0, \tag{56}$$

and by the second law of thermodynamics

$$S_t + \left(\frac{Q}{\theta} + J\right)_x \geq 0. \tag{57}$$

Here σ is the one-dimensional stress, v is the particle velocity, Q is the heat flux, E is the internal energy, S is the entropy, θ is temperature, J is the extra entropy flux, subscripts denote derivatives.

The canonical energy equation is derived from Eq. (56) by introducing the free energy per unit volume $W := E - S\theta$ and taking into account the balance of linear momentum (55)

$$(S\theta)_t + Q_x = h^{int}, \quad h^{int} := \sigma\varepsilon_t - W_t. \tag{58}$$

Multiplying Eq. (55) by u_x we then check that Eq. (55) yields the following canonical balance of material momentum (cf. [36])

$$P_t - b_x = f^{int} + f^{inh}, \tag{59}$$

where the material momentum P, the material Eshelby stress b, the material inhomogeneity force f^{inh}, and the material internal force f^{int} are defined by [36]

$$P := -\rho_0 u_t u_x, \quad b := -\left(\frac{1}{2}\rho_0 v^2 - W + \sigma\varepsilon\right), \tag{60}$$

$$f^{inh} := \left(\frac{1}{2}v^2\right)(\rho_0)_x - \left.W_x\right|_{expl}, \quad f^{int} := \sigma u_{xx} - \left.W_x\right|_{impl}. \tag{61}$$

In the case of non-zero extra entropy flux, the second law of thermodynamics gives

$$-\left(W_t + S\theta_t\right) + \sigma\varepsilon_t + (\theta J)_x - \left(\frac{Q}{\theta} + J\right)\theta_x \geq 0, \tag{62}$$

where $\varepsilon = u_x$ is the one-dimensional strain measure.

5.1 Dual internal variables

Now we suppose that the free energy depends on the internal variables φ, ψ and their space derivatives $W = \overline{W}(u_x, \theta, \varphi, \varphi_x, \psi, \psi_x)$. Then the constitutive equations follow

$$\sigma := \frac{\partial \overline{W}}{\partial u_x}, \quad S = -\frac{\partial \overline{W}}{\partial \theta}, \quad \tau := -\frac{\partial \overline{W}}{\partial \varphi}, \quad \eta := -\frac{\partial \overline{W}}{\partial \varphi_x}, \\ \xi := -\frac{\partial \overline{W}}{\partial \psi}, \quad \zeta := -\frac{\partial \overline{W}}{\partial \psi_x}. \tag{63}$$

We include into consideration the non-zero extra entropy flux according to Eq. (35)

$$J = -\theta^{-1}\eta\varphi_t - \theta^{-1}\zeta\psi_t. \tag{64}$$

The canonical equations of momentum and energy follow as

$$P_t - \widetilde{b}_x = f^{th} + \widetilde{f}^{intr}, \tag{65}$$

$$(S\theta)_t + \widetilde{Q}_x = h^{th} + \widetilde{h}^{intr}, \tag{66}$$

with appropriate modifications

$$\begin{aligned} \widetilde{b} &= -\left(\frac{1}{2}\rho_0 v^2 - W + \sigma u_x - \eta\varphi_x - \zeta\psi_x\right), \\ \widetilde{Q} &= Q - \eta\varphi_t - \zeta\psi_t, \end{aligned} \tag{67}$$

where thermal and intrinsic source terms are determined as follows

$$\begin{aligned} f^{th} &:= S\theta_x, \quad \widetilde{f}^{intr} := (\tau - \eta_x)\varphi_x + (\xi - \zeta_x)\psi_x \\ h^{th} &:= S\theta_t, \quad \widetilde{h}^{intr} := (\tau - \eta_x)\varphi_t + (\xi - \zeta_x)\psi_t. \end{aligned} \tag{68}$$

The latter means that the dissipation inequality reduces to

$$\Phi = (\tau - \eta_x)\varphi_t + (\xi - \zeta_x)\psi_t - \left(\frac{Q - \eta\varphi_t - \zeta\psi_t}{\theta}\right)\theta_x \geq 0. \tag{69}$$

If we assume that intrinsic dissipation is still independent of temperature gradient, then we are forced to modify the Fourier's law

$$Q - \eta\varphi_t - \zeta\psi_t = -k\theta_x, \tag{70}$$

to satisfy the thermal part of the dissipation inequality.

The remaining intrinsic part of the dissipation inequality (69) can be satisfied by several means. We consider three main cases for choosing the evolution equations for internal variables:

1. non-dissipative case (internal variables contribute only to the reversible part of the metriplectic structure (50));
2. fully dissipative case (internal variables contribute only to the irreversible dissipative part of the metriplectic structure (50));
3. intermediate case (internal variables contribute to both the reversible and the irreversible dissipative parts).

It is easy to see, that the choice

$$\varphi_t = R(\xi - \zeta_x), \quad \psi_t = -R(\tau - \eta_x), \tag{71}$$

where R is an appropriate constant, leads to zero intrinsic dissipation, because in this case the first two terms in the right-hand side of the dissipation inequality (69) cancel one another. In this **non-dissipative** case the two evolution equations (71) express the duality between internal variables: one internal variable is driven by another one and vice versa [32, 33]. The corresponding conductivity matrix $\mathbf{R}$ is antisymmetric.

The **fully dissipative** case corresponds to the choice of evolution equations in the form

$$\varphi_t = R_1(\tau - \eta_x), \quad R_1 > 0, \quad \psi_t = R_2(\xi - \zeta_x), \quad R_2 > 0. \tag{72}$$

In this case the intrinsic dissipation is always non-negative, because it consists in a linear combinations of squares with positive coefficients. Accordingly, the conductivity matrix $\mathbf{R}$ is a diagonal one.

At last, the **intermediate** case is achieved by the choice

$$\varphi_t = R(\xi - \zeta_x), \quad \psi_t = -R(\tau - \eta_x) + R_2(\xi - \zeta_x). \tag{73}$$

Here the intrinsic dissipation is partly canceled, as in the non-dissipative case, and its remaining part is the square with a positive coefficient.

To see the difference in the choice of the evolution equations for internal variables in more detail, let us derive field equations. Using a quadratic function as the free energy dependence

$$\begin{aligned}\overline{W} =& \frac{1}{2}\left(\lambda+2\mu\right)u_x^2 - \frac{\rho_0 c}{2\theta_0}\left(\theta-\theta_0\right)^2 + m\left(\theta-\theta_0\right)u_x + \\ &+ A\varphi u_x + A'\varphi_x u_x + \frac{1}{2}B\varphi^2 + \frac{1}{2}C\varphi_x^2 + \frac{1}{2}D\psi^2,\end{aligned} \tag{74}$$

we include for simplicity only the contribution of the second internal variable itself, like it was in the isothermal case [32, 33]. Here the thermoelastic coefficient m is related to the dilatation coefficient α, and the Lamé coefficients λ and μ by $m = \alpha(3\lambda + 2\mu)$. In this case, the stresses are determined as follows:

$$\sigma = \left(\lambda+2\mu\right)u_x + m\left(\theta-\theta_0\right) + A\varphi + A'\varphi_x, \quad \eta = -C\varphi_x - A'u_x, \tag{75}$$

and τ coincides with the interactive internal force

$$\tau = -\frac{\partial\overline{W}}{\partial\varphi} = -Au_x - B\varphi. \tag{76}$$

The terms related to the second internal variable are

$$\zeta = -\frac{\partial\overline{W}}{\partial\psi_x} = 0, \quad \xi = -\frac{\partial\overline{W}}{\partial\psi} = -D\psi. \tag{77}$$

5.1.1 The non-dissipative case

In the non-dissipative case, it follows from Eqs. (71) and (77) that

$$\varphi_t = -RD\psi, \tag{78}$$

i.e., the dual internal variable ψ is proportional to the time derivative of the primary internal variable φ_t. It follows immediately from Eq. (78) that the evolution equation for the dual internal variable $(71)_2$ can be rewritten in terms of the primary one as a hyperbolic equation

$$\varphi_{tt} = R^2 D(\tau - \eta_x). \tag{79}$$

As a result, we can represent the equations of motion in the form, which includes only the primary internal variable

$$\begin{aligned} u_{tt} &= (\lambda + 2\mu)\, u_{xx} + m\theta_x + A\varphi_x + A'\varphi_{xx}, \\ I\varphi_{tt} &= C\varphi_{xx} + A'u_{xx} - Au_x - B\varphi, \end{aligned} \tag{80}$$

where $I = \frac{1}{R^2 D}$ is an internal inertia measure.

Accounting for the modified Fourier's law (70), we can represent the energy conservation equation (66) for small deviations from θ_0 in its classical form

$$\rho_0 c\, \theta_t - (k\theta_x)_x = m\theta_0 u_{xt}. \tag{81}$$

This means that in this non-dissipative case the internal variables do not appear in the heat conduction equation. At the same time the internal variables change the heat flux because of the modified Fourier's law (70). If we identify the primary internal variable with a microdeformation, then we arrive at the thermoelastic extension of the model of linear dispersive wave propagation in solids with a microstructure [33].

5.1.2 The fully dissipative case

In the fully dissipative case, the balance of linear momentum has the same form as previously

$$u_{tt} = (\lambda + 2\mu)\, u_{xx} + m\theta_x + A\varphi_x + A'\varphi_{xx}, \tag{82}$$

but the evolution equations (72) take on the form

$$\varphi_t = R_1(\tau - \eta_x) = R_1\left(C\varphi_{xx} + A'u_{xx} - Au_x - B\varphi\right), \tag{83}$$

$$\psi_t = R_2(\xi - \zeta_x) = -R_2 D\psi. \tag{84}$$

The energy conservation equation (66) according to the modified Fourier's law (70) takes the following form for small deviations from θ_0

$$\rho_0 c\,\theta_t - (k\theta_x)_x = m\theta_0 u_{xt} + \frac{1}{R_1}\varphi_t^2 + \frac{1}{R_2}\psi_t^2, \tag{85}$$

because the intrinsic dissipation is non-zero.

The evolution equations for the primary and secondary internal variables (Eqs. (83) and (84)) differ from each other only due to the specific choice of the free energy dependence (74). If we introduce a similar dependence for both internal variables, then the corresponding evolution equations will be also similar. This means that in the fully dissipative case we have no need for the dual internal variables. The conventional single internal variable theory [29, 30] is sufficient. Since we are interested in the influence of temperature gradients, we may expect that the free energy depends only on the gradient of the primary internal variable, but not on the variable itself. In the simplest case, this corresponds to the choice of coefficients $A = 0, B = 0, D = 0$ in Eq. (74). Then equations of motion and energy are reduced to

$$u_{tt} = (\lambda + 2\mu)\, u_{xx} + m\theta_x + A'\varphi_{xx}, \tag{86}$$

$$\varphi_t = R_1 C\varphi_{xx} + A' u_{xx}, \tag{87}$$

$$\rho_0 c\,\theta_t - (k\theta_x)_x = m\theta_0 u_{xt} + \frac{1}{R_1}\varphi_t^2. \tag{88}$$

The evolution equation for the primary internal variable (87) becomes the parabolic one and we can identify the internal variable with a microtemperature. Its influence on the macrotemperature manifests itself in the source term in the right hand side of Eq. (88). The microtemperature (and its gradient) can be non-zero even in the case of zero initial and boundary conditions for them due to the coupling with the equation of motion.

5.1.3 The intermediate case

In the intermediate case, we have again for the primary variable

$$\varphi_t = -RD\psi, \tag{89}$$

and the evolution equation for the secondary internal variable

$$\psi_t = -R(\tau - \eta_x) + R_2(\xi - \zeta_x), \tag{90}$$

is represented as

$$-\frac{1}{RD}\varphi_{tt} = -R(C\varphi_{xx} + A'u_{xx} - Au_x - B\varphi) + \frac{R_2}{R}\varphi_t, \tag{91}$$

or in the following form

$$I\varphi_{tt} + \frac{R_2}{R^2}\varphi_t = (C\varphi_{xx} + A'u_{xx} - Au_x - B\varphi), \tag{92}$$

which is a Cattaneo-Vernotte-type hyperbolic equation [7] for the primary internal variable φ.

Correspondingly, the energy conservation equation (66) in this case has the form

$$\rho_0 c\,\theta_t - (k\theta_x)_x = m\theta_0 u_{xt} + R_2 D^2 \varphi_t^2. \tag{93}$$

As in the previous case, the equation for the macrotemperature (93) is influenced by a source term which depends on the internal variable. Let us consider again the case when the free energy depends only on the gradient of the primary internal variable, but not on the variable itself. This case corresponds to the choice of coefficients $A = 0, B = 0$. The reduced equations of motion are coupled

$$u_{tt} = (\lambda + 2\mu)\,u_{xx} + m\theta_x + A'\varphi_{xx}, \tag{94}$$

$$I\varphi_{tt} + \frac{R_2}{R^2}\varphi_t = (C\varphi_{xx} + A'u_{xx}), \tag{95}$$

which means that the primary internal variable possesses a wave-like behavior induced by macrodeformation. Identifying the internal variable with the microtemperature, we see that the microtemperature may induce the wave-like propagation also for the macrotemperature. As in the previous case, non-zero solutions for the primary internal variable are provided by the coupling with the balance of linear momentum even if initial and boundary conditions are zero for the internal variable.

6 Conclusions

Comparing the Cattaneo relation for the heat flux [7]

$$t_0 \frac{\partial Q}{\partial t} + Q = -k \nabla \theta, \tag{96}$$

with modified Fourier's law arising from the dual internal variables theory

$$Q - \eta \varphi_t - \zeta \psi_t = -k \theta_x, \tag{97}$$

we can see that formally they can be identified under the choice

$$\varphi = Q, \quad \eta = -t_0, \quad \zeta = 0. \tag{98}$$

Moreover, the Jeffreys-type relation [7]

$$t_0 \frac{\partial Q}{\partial t} + Q = -k \nabla \theta - t_1 k_1 \frac{\partial \nabla \theta}{\partial t}, \tag{99}$$

can also be retrieved by

$$\varphi = Q, \quad \eta = -t_0, \quad \psi = \theta_x, \quad \zeta = -t_1 k_1. \tag{100}$$

However, we cannot identify internal variables with macroscopic fluxes and gradients, which can be controlled by external boundary conditions. Even if this can be done formally, then the macroscopic heat equation cannot be changed significantly in the dual internal variables theory, because the modified heat flux in the energy conservation equation coincides with that in the dissipation inequality. By contrast, the Cattaneo relation or the Jeffreys relation modifies the heat flux independently of that in the energy conservation equation [8].

Thus, the dual internal variables approach provides several possibilities for evolution equations for internal variables. Accordingly, the internal variables can describe effects of microdeformations or microtemperatures (and their gradients). The corresponding evolution equations can be hyperbolic even for microtemperatures, which in its turn can induce wave-like propagation for macrotemperature due to the coupling of equations.

The overall description of thermomechanical processes in microstructured solids includes both direct and indirect couplings of equations of motion and heat conduction at the macrolevel. In addition to the conventional direct coupling, there exists the coupling between macromotion and microtemperature evolution. This means that the macrodeformation can induce microtemperature perturbations 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.

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