Thermomechanical Multiscale Constitutive Modeling: Accounting for Microstructural Thermal Effects

Pablo J. Blanco & Sebastián M. Giusti

Journal of Elasticity
The Physical and Mathematical Science of Solids

ISSN 0374-3535

J Elast
DOI 10.1007/s10659-013-9445-2

J Elast
DOI 10.1007/s10659-013-9445-2

Thermomechanical Multiscale Constitutive Modeling: Accounting for Microstructural Thermal Effects

Pablo J. Blanco · Sebastián M. Giusti

Received: 4 September 2012

Abstract In this work we present a thermomechanical multiscale constitutive model for materials with microstructure. In these materials thermal effects at microscale have an impact on the effective macroscopic stress. As a result, it turns out that the homogenized stress depends upon the macroscopic temperature and its gradient. In order to allow this interplay to be thermodynamically valid, we resort to a macroscopic extended thermodynamics whose elements are derived from the microscopic behavior using homogenization concepts. Hence, the thermodynamics implications of this new class of multiscale models are discussed. A variational approach based on the Hill–Mandel Principle of Macro-homogeneity, and which makes use of the volume averaging concept over a local representative volume element (RVE), is employed to derive the thermal and mechanical equilibrium problems at the RVE level and the corresponding homogenization expressions for the effective heat flux and stress. The material behavior at the RVE level is described through standard phenomenological constitutive models. To sum up, the novel contribution of the model presented here is that it allows to include the microscopic temperature fluctuation field, obtained from the multiscale thermal analysis, in the micro-mechanical problem at the RVE level while keeping thermodynamic consistency.

Keywords Multiscale modeling · Elasticity tensor · Thermal conductivity tensor · Thermal expansion tensor · Non-standard thermodynamics

Mathematics Subject Classification 49S05 · 74A20 · 74A60 · 74Q15

P.J. Blanco (✉)
Laboratório Nacional de Computação Científica LNCC/MCTI, Av. Getúlio Vargas 333,
25651-075 Petropolis, Brazil
e-mail: pjblanco@lncc.br

S.M. Giusti
Facultad Regional Córdoba UNT/FRC-CONICET, Universidad Tecnológica Nacional, Maestro
M. López esq. Cruz Roja Argentina, X5016ZAA, Cordoba, Argentina
e-mail: sgiusti@civil.frc.utn.edu.ar

Published online: 16 May 2013

1 Introduction

The constitutive modeling of solids based on multiscale theories has become the subject of intensive research in applied and computational mechanical sciences. The growing interest in constitutive modeling by multiscale techniques has two important motivations, the first is the current need for more accurate constitutive models, and the second is related to the limit of the descriptive/predictive capability of conventional phenomenological continuum models. One important example of these facts is the mathematical modeling of biological tissue. The typical microstructure of biological material can be extremely elaborated, resulting in a macroscopic constitutive response of difficult representation by means of conventional phenomenological constitutive models [5, 35]. Often, the modeling of such phenomena through a single—macroscopic—scale approach results in important discrepancies between the predicted and observed constitutive responses.

Classical multiscale models have been derived from the analysis of partial differential equations [1, 33]. These models are based on the construction of the solution of the system of PDEs by means of an asymptotic expansion in terms of a small parameter ε, which is the ratio between the characteristic lengths of both scales. Then, the problems associated to each power of ε of this expansion are derived. Each one of these problems are referred to a scale of the multiscale formulation. The key of the method relies in the proof of the convergence of the asymptotic expansion when the system of PDEs at the different scales is identified. Particularly, the thermomechanical multiscale problem has been studied using this classical approach in [7, 11, 12, 34]. In these works it is shown that the mechanical problem at the microscopic scale depends exclusively on the macroscopic strain and on the macroscopic temperature field. This means that the fluctuations of the microscopic temperature field, which are obtained after solving the thermal problem at the RVE level, do not have effect neither in the problem for the microscopic mechanical problem nor in the obtained effective stress. This is a consequence of the specific technique—asymptotic analysis—used in the derivation of this class of multiscale models. Thus, the *scales-separation* concept has been employed as an argument in the derivation of variational multiscale techniques that proposed thermomechanical constitutive models in order to disregard the effect of the microscopic temperature fluctuations in the micro-mechanical problem. For instance, in [7, 36, 37], the homogenized thermal expansion tensor depends on the solution of a micro-mechanical problem which is, in turn, related to the macroscopic strain and *just* to the macroscopic temperature.

On the other hand, in thermomechanical problems, materials with inner structure pose the difficulty of accommodating the complex interplay between mechanical and thermal microstructural phenomena within the same framework. To address this problem, several approaches have been proposed: from micromorphic materials with thermal effects [3, 15, 23, 28, 29, 31, 32] to second-grade continua [4, 8–10] and models based on extended thermodynamics [17, 24, 25] as well as other alternatives accounting for microstructure features at the macroscale [30]. In all these approaches, constitutive models are able to account for the effects of temperature gradients in the stress state. This is possible since the thermodynamics is somehow consistently generalized to take into account this dependence. Using a different approach, the effect of microtemperatures in the two-dimensional plane thermoelasticity problem has been recently addressed in [2].

In the context of constitutive multiscale analysis, as stated in [36], the fact of sticking to the classical thermodynamics at the macroscale has strong consequences in the way in which thermal effects can be accounted for in a micro-mechanical equilibrium problem. As an example of this fact, we refer to the problem of the microscopic thermal fluctuation in a multiscale thermal analysis. According to [36] (see also [26, 38]), the thermomechanical problem at the microscale cannot incorporate the thermal fluctuations obtained from a multiscale thermal analysis. Therefore, the mean value of the macroscopic temperature is exclusively responsible for introducing the thermal contribution in the microscopic mechanical problem. Hence, the classical thermodynamics still holds at the macroscopic problem and all the classical constitutive dependencies of free energy, heat flux and stress state upon temperature, temperature gradient and strain are valid.

The contribution of this work is the development of a multiscale variational framework that permits to incorporate the microscopic thermal fluctuations in the micro-mechanical analysis. As a consequence, this yields a dependence of the macroscopic stress state upon the macroscopic temperature gradient. We assume that the classical thermodynamics holds at the microscale (classical Clausius–Duhem inequality), from which classical thermomechanical constitutive models are proposed at the RVE level. The present model is then formulated using just two basic concepts: (i) homogenization (volume averaging) of microscopic temperature, microscopic temperature gradient and microscopic strain; and (ii) the Hill–Mandel Principle of Macro-homogeneity (multiscale virtual power balance). Then, the thermomechanical coupling between the micro-strain and micro-temperature fields naturally leads to a dependence of the macroscopic stress upon the three macroscopic quantities: strain, temperature and temperature gradient. Since this functional dependence with respect to the temperature gradient is not allowed in the classical thermodynamics setting, an extended macroscopic thermodynamics is mandatory to accommodate this more complex material behavior (non-classical Clausius–Duhem inequality). Therefore, definitions of the macroscopic internal energy, entropy and entropy vector are introduced, following [24]. Notice that material modeling considered this way leads to a sort of second grade continua which accounts for temperature gradient effects on the macroscopic stress state. In the present model the temperature fluctuations considered in the micro-thermal problem are the same temperature fluctuations considered in the micro-mechanical problem. In this sense, the microscopic temperature field is unique within the entire analysis. This is different from [36], where the authors resort to the argument of scales separation in order to neglect the temperature fluctuations in the micro-mechanical problem.

The paper is organized as follows: in Sect. 2 we introduce some preliminary concepts in the multiscale analysis. Section 3 recalls the formulation of the macroscopic thermomechanical problem. The multiscale thermal analysis is introduced in Sect. 4. The constitutive multiscale framework for the thermomechanical analysis is presented in Sect. 5. In Sect. 6 we present the extended macroscopic thermodynamics derived from the developed multiscale model. Finally, some concluding remarks are outlined in Sect. 7.

2 Preliminaries in the Multiscale Analysis

As stated in the Introduction Section we follow a purely variational approach to derive the thermomechanical constitutive multiscale model. The Hill–Mandel Macro-homogeneity principle is the underlying variational principle that provides the multiscale virtual power balance. This variational problem is closed by providing kinematical restrictions which are derived from the concept of volume averaging in the Representative Volume Element (RVE) [18]. See Sect. 4 for the constitutive thermal analysis and Sect. 5 for the constitutive mechanical analysis. This constitutive modeling approach follows closely the strategy presented in

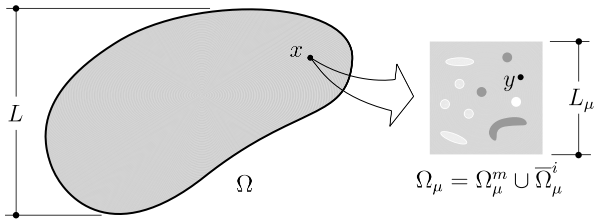

Fig. 1 Macroscopic continuum with a locally attached microstructure featuring thermal and mechanical effects

[13, 20, 21], whose variational structure is described in detail in [6, 27]. In this context, the main concept is the assumption that any point $\mathbf{x}$ of the macroscopic continuum (refer to Fig. 1) is associated to a local RVE, with domain Ω_μ and boundary $\partial\Omega_\mu$, which has a characteristic length L_μ, much smaller than the characteristic length L of the macro-continuum domain, $\Omega \subset \mathbb{R}^n$ for $n = 2$ or 3. For simplicity, we consider that the RVE domain consists of a matrix Ω_μ^m, containing inclusions of different materials occupying a domain Ω_μ^i (see Fig. 1), but the formulation is completely analogous to the one presented here if the RVE contains voids instead. Hereafter, symbols $(\cdot)_\mu$ denote quantities associated to the microscale.

In order to not obscure the underlying concepts, in the next two sections we work with the mechanical multiscale model under the hypothesis of infinitesimal strains. Also, the classical thermomechanical analysis is considered, recalling that this entails a one-way coupling, i.e., the temperature has an effect on the stress state, but strain rates do not affect the thermal state of the body.

As in any thermomechanical problem, the primal variables that define the thermodynamical state of the body at the macroscopic scale are the temperature θ, the temperature gradient $\mathbf{g} = \nabla\theta$, and the strain tensor $\boldsymbol{\varepsilon}$. Therefore, proper homogenization formulas for these three quantities are mandatory for the well-posedness of the problem. The idea of the variational formulation presented in the following sections lies on top of this fundamental concept. As an outcome, the dual thermodynamical variables will be the heat flux $\mathbf{q}$ and the stress tensor $\boldsymbol{\sigma}$, as shown in the corresponding sections.

Since it will be clear from the context, in what follows we will not differentiate between the gradient with respect to macroscopic coordinates $\mathbf{x}$ and the gradient with respect to microscopic coordinates $\mathbf{y}$. Both will be simply denoted by the symbol ∇.

3 Macroscopic Thermomechanical Problem

At the macroscale, we consider the thermomechanical analysis in the steady state setting. Therefore, the problem entails obtaining the temperature and displacement fields over Ω. The thermomechanical equilibrium problem is formulated in a variational context. The first step consists of introducing the affine spaces of kinematically admissible temperature and displacement fields at the macroscale. These sets are, respectively,

$$\begin{aligned} \Theta &:= \{\theta \in H^1(\Omega) : + \text{ essential thermal b.c.}\}, \\ \mathcal{U} &:= \{\mathbf{u} \in \mathbf{H}^1(\Omega) : + \text{ essential mechanical b.c.}\}. \end{aligned} \tag{1}$$

Therefore, the spaces of admissible temperature and displacement variations are defined, respectively, as

$$\begin{aligned} \widehat{\Theta} &:= \left\{\theta \in H^1(\Omega) : + \text{homogeneous essential thermal b.c.}\right\}, \\ \widehat{\mathcal{U}} &:= \left\{\mathbf{u} \in \mathbf{H}^1(\Omega) : + \text{homogeneous essential mechanical b.c.}\right\}. \end{aligned} \tag{2}$$

Hence, the macroscopic thermal variational problem reads: given the thermal source f and proper natural thermal boundary conditions, find $\theta \in \Theta$ such that the heat flux $\mathbf{q}$ is such that

$$\int_\Omega \mathbf{q} \cdot \nabla\hat{\theta}\, dV = \int_\Omega f\hat{\theta}\, dV + \text{ natural thermal b.c.}, \quad \forall\hat{\theta} \in \widehat{\Theta}. \tag{3}$$

In the same manner, the macroscopic mechanical variational problem is: given the temperature field θ satisfying (3), the loading $\mathbf{f}$ and proper natural mechanical boundary conditions, find $\mathbf{u} \in \mathcal{U}$ such that the stress state $\boldsymbol{\sigma}$ is such that

$$\int_\Omega \boldsymbol{\sigma} \cdot \nabla^s\hat{\mathbf{u}}\, dV = \int_\Omega \mathbf{f} \cdot \hat{\mathbf{u}}\, dV + \text{ natural mechanical b.c.}, \quad \forall\hat{\mathbf{u}} \in \widehat{\mathcal{U}}. \tag{4}$$

Variational problems (3) and (4) are closed once the functional dependencies of the heat flux $\mathbf{q}$ and the stress state $\boldsymbol{\sigma}$ are given in terms of the macroscopic temperature field θ, macroscopic temperature gradient $\mathbf{g}$, and of the macroscopic strain field $\boldsymbol{\varepsilon}$. These functional dependencies will be obtained exploiting the multiscale analysis in the following sections. Specifically, an effective heat flux will be obtained from the thermal multiscale analysis (see Sect. 4) and an effective stress will be computed from the mechanical multiscale analysis with thermal effects (see Sect. 5).

4 Multiscale Thermal Analysis

In order to make the work self-contained, and to work with a unified notation, in this section we present the basic ideas behind the multiscale thermal problem.

4.1 Kinematical Admissibility

In the context of the previous section we consider that at any arbitrary point $\mathbf{x} \in \Omega$, the macroscopic temperature gradient $\mathbf{g}$ is the volume average of the microscopic temperature gradient $\nabla\theta_\mu$:

$$\mathbf{g} = \frac{1}{V_\mu}\int_{\Omega_\mu} \nabla\theta_\mu\, dV, \tag{5}$$

where θ_μ denotes the microscopic absolute temperature field and V_μ is the total volume of the RVE. As stated before, since we are in a thermomechanics setting in which the temperature itself has a physical relevance for the mechanical problem, we also consider the following homogenization formula for the temperature

$$\theta = \frac{1}{V_\mu}\int_{\Omega_\mu} \theta_\mu\, dV. \tag{6}$$

By making use of Green's theorem, we can promptly establish that the averaging relation (5) is equivalent to the following constraint on the temperature field of the RVE:

$$\int_{\partial\Omega_\mu} \theta_\mu \mathbf{n}\, dS = V_\mu \mathbf{g}, \tag{7}$$

where $\mathbf{n}$ is the unit outward vector to $\partial\Omega_\mu$.

Now, without loss of generality, the microscopic temperature field θ_μ can be split into a sum of the macroscopic temperature field θ, the contribution of the macroscopic temperature gradient field $\mathbf{g}$, and a microscopic temperature fluctuation field, $\tilde{\theta}_\mu(\mathbf{y})$

$$\theta_\mu(\mathbf{y}) = \theta + \mathbf{g}\cdot(\mathbf{y}-\mathbf{y}_o) + \tilde{\theta}_\mu(\mathbf{y}), \tag{8}$$

where $\mathbf{y}_o$ is

$$\mathbf{y}_o = \frac{1}{V_\mu}\int_{\Omega_\mu} \mathbf{y}\, dV. \tag{9}$$

Introducing the above splitting in (6) we obtain the following constraint for the microscopic temperature fluctuation field:

$$\int_{\Omega_\mu} \tilde{\theta}_\mu\, dV = 0. \tag{10}$$

In view of the splitting (8), and taking into account constraints (5) and (6) we define the minimally constrained space of admissible microscopic temperature fluctuation fields at the RVE

$$\Theta_\mu := \left\{\theta_\mu \in H^1(\Omega_\mu) : \int_{\Omega_\mu} \theta_\mu\, dV = 0, \int_{\partial\Omega_\mu} \theta_\mu \mathbf{n}\, dS = \mathbf{0}\right\}. \tag{11}$$

Therefore, the resulting space of admissible variations of the microscopic temperature field at the RVE is also Θ_μ.

Remark 1 Note that other multiscale models could be obtained by considering any other space of admissible functions, say Θ_μ^X. It is just necessary that $\Theta_\mu^X \subset \Theta_\mu$. An instance of an alternative is the classical model with periodic boundary conditions. For a more detailed description on this topic, we refer the reader to [6, 27].

Taking the gradient with respect to the microscopic coordinates $\mathbf{y}$ in (8), yields the microscopic temperature gradient

$$\nabla\theta_\mu = \mathbf{g} + \nabla\tilde{\theta}_\mu, \tag{12}$$

which is the sum of a homogeneous gradient (uniform over the RVE) coinciding with the macroscopic temperature gradient and the field $\nabla\tilde{\theta}_\mu$ corresponding to a fluctuation of the microscopic temperature gradient around the homogenized value.

4.2 The Hill–Mandel principle and its variational consequences

Another fundamental concept underlying multiscale models of the present type is the *Hill–Mandel Principle of Macro-homogeneity*. Here, we shall assume the analogous relation for the thermal case [13, 14]

$$\mathbf{q}\cdot\hat{\mathbf{g}} = \frac{1}{V_\mu}\int_{\Omega_\mu} \mathbf{q}_\mu(\theta_\mu)\cdot\nabla\hat{\theta}_\mu\, dV \quad \forall(\hat{\theta}_\mu, \hat{\mathbf{g}}) \text{ kinematically admissible,} \tag{13}$$

where $\mathbf{q}_\mu(\theta_\mu)$ denotes the microscopic heat flux associated to the microscopic temperature θ_μ. Exploiting relation (8) in (13), leads to the following variational problem: given the macroscopic temperature θ and the macroscopic temperature gradient $\mathbf{g}$, find $\mathbf{q}$ and $\tilde{\theta}_\mu \in \Theta_\mu$ such that

$$\mathbf{q}\cdot\hat{\mathbf{g}} = \frac{1}{V_\mu}\int_{\Omega_\mu} \mathbf{q}_\mu\big(\theta + \mathbf{g}\cdot(\mathbf{y}-\mathbf{y}_o) + \tilde{\theta}_\mu\big)\cdot(\hat{\mathbf{g}} + \nabla\hat{\tilde{\theta}}_\mu)\, dV, \quad \forall\hat{\tilde{\theta}}_\mu \in \Theta_\mu \text{ and } \forall\hat{\mathbf{g}}. \tag{14}$$

Equation (13) plays a crucial role in the formulation of heat conduction constitutive models within the present framework since it provides the variational principle that governs the scale bridging for the thermal problem.

Now we derive the consequences using standard variational arguments. Basically they stand for the homogenization formula for the heat flux and the microscopic thermal equilibrium problem.

Micro-thermal equilibrium problem: Considering $\hat{\mathbf{g}} = 0$ in (14) leads to the microscopic thermal equilibrium problem: given the macroscopic temperature θ and the macroscopic temperature gradient $\mathbf{g}$, find the temperature fluctuation field $\tilde{\theta}_\mu \in \Theta_\mu$ such that

$$\int_{\Omega_\mu} \mathbf{q}_\mu\big(\theta + \mathbf{g}\cdot(\mathbf{y}-\mathbf{y}_o) + \tilde{\theta}_\mu\big)\cdot\nabla\hat{\tilde{\theta}}_\mu\, dV = 0, \quad \forall\hat{\tilde{\theta}}_\mu \in \Theta_\mu. \tag{15}$$

Characterization of the macroscopic heat flux: Considering now $\hat{\tilde{\theta}}_\mu = 0$ in (14) results the characterization of the macroscopic heat flux vector $\mathbf{q}$: given the macroscopic temperature θ, its gradient $\mathbf{g}$, and $\tilde{\theta}_\mu$—the solution of problem (15)—, compute $\mathbf{q}$ as

$$\mathbf{q} = \frac{1}{V_\mu}\int_{\Omega_\mu} \mathbf{q}_\mu\big(\theta + \mathbf{g}\cdot(\mathbf{y}-\mathbf{y}_o) + \tilde{\theta}_\mu\big)\, dV. \tag{16}$$

In the present analysis, we shall assume that the materials of the RVE matrix and inclusions satisfy the classical Fourier constitutive law:

$$\mathbf{q}_\mu(\xi) = -\mathbf{K}_\mu\nabla\xi, \tag{17}$$

where $\mathbf{K}_\mu$ is the second order thermal conductivity tensor of the RVE (which is admitted to be positive definite, i.e. $\mathbf{K}_\mu\mathbf{v}\cdot\mathbf{v} > 0\ \forall\mathbf{v} \neq 0$ and $\mathbf{K}_\mu\mathbf{v}\cdot\mathbf{v} = 0$ if and only if $\mathbf{v}$ is the null vector field). The above linear relation together with the additive decomposition (8) allows the microscopic thermal flux field to be split as

$$\mathbf{q}_\mu(\theta_\mu) = -\mathbf{K}_\mu\mathbf{g} - \mathbf{K}_\mu\nabla\tilde{\theta}_\mu. \tag{18}$$

By introducing decomposition (18) into the thermal equilibrium equation (15), we obtain the closed form of the microscopic thermal equilibrium problem: given $\mathbf{g}$, find $\tilde{\theta}_\mu \in \Theta_\mu$ such that

$$\int_{\Omega_\mu} \mathbf{K}_\mu\nabla\tilde{\theta}_\mu\cdot\nabla\hat{\tilde{\theta}}_\mu\, dV = -\int_{\Omega_\mu} \mathbf{K}_\mu\mathbf{g}\cdot\nabla\hat{\tilde{\theta}}_\mu\, dV, \quad \forall\hat{\tilde{\theta}}_\mu \in \Theta_\mu, \tag{19}$$

and the homogenization formula for the macroscopic heat flux results

$$\mathbf{q} = -\left(\frac{1}{V_\mu}\int_{\Omega_\mu} \mathbf{K}_\mu \, dV\right)\mathbf{g} - \frac{1}{V_\mu}\int_{\Omega_\mu} \mathbf{K}_\mu \nabla\tilde{\theta}_\mu \, dV. \tag{20}$$

From (20) and (19) it is clear that $\mathbf{q}$ depends linearly on $\mathbf{g}$ and the characterization of this linear operator (homogenized macro thermal conductivity tensor) is described next.

4.3 The Homogenized Thermal Conductivity Tensor

Crucial to the developments of the multiscale model for the macroscopic thermal problem is the derivation of formulae for the macroscopic heat conductivity tensor. This is addressed in the following.

To obtain the tangent operator from (20) we derive (19) with respect to $\mathbf{g}$. Calling $\mathbf{d_g} := \frac{\partial\tilde{\theta}_\mu}{\partial \mathbf{g}}$ (a vector field), and denoting $[\mathbf{d_g}]_i = \mathbf{d_g}\cdot\mathbf{e}_i$ (a scalar field)—being $\mathbf{e}_i$ the unit Cartesian vectors—the variational equation for the tangent field is written as: find $[\mathbf{d_g}]_i \in \Theta_\mu$, such that

$$\int_{\Omega_\mu} \mathbf{K}_\mu \nabla[\mathbf{d_g}]_i \cdot \nabla\hat{\tilde{\theta}}_\mu \, dV = -\int_{\Omega_\mu} \mathbf{K}_\mu \mathbf{e}_i \cdot \nabla\hat{\tilde{\theta}}_\mu \, dV, \quad \forall\hat{\tilde{\theta}}_\mu \in \Theta_\mu, \tag{21}$$

for $i = 1, \ldots, n$.

Now, from the additive splitting of the microscopic temperature field (8), the homogenization procedure for the heat flux (16) and by using the solution of (21), we have that the macroscopic conductivity tensor can be obtained as the sum

$$-\frac{\partial \mathbf{q}}{\partial \mathbf{g}} := \mathbf{K} = \overline{\mathbf{K}} + \widetilde{\mathbf{K}}, \tag{22}$$

of a homogenized (volume average) macroscopic conductivity tensor $\overline{\mathbf{K}}$, given by,

$$\overline{\mathbf{K}} = \frac{1}{V_\mu}\int_{\Omega_\mu} \mathbf{K}_\mu \, dV, \tag{23}$$

and a contribution $\widetilde{\mathbf{K}}$ associated to the microscopic temperature fluctuation field defined, from (21), as

$$\widetilde{\mathbf{K}} = \left[\frac{1}{V_\mu}\int_{\Omega_\mu} \left(\mathbf{K}_\mu \nabla[\mathbf{d_g}]_j\right)_i dV\right](\mathbf{e}_i \otimes \mathbf{e}_j). \tag{24}$$

For a more detailed description on the derivation of the above expressions, we refer the reader to [14, 20].

Although it is not needed in the thermal analysis, we are interested in checking that the tangent operator with respect to the macroscopic temperature is zero. That is, by deriving (19) with respect to θ and calling $d_\theta := \frac{\partial\tilde{\theta}_\mu}{\partial\theta}$ (a scalar field), we obtain the variational equation for this tangent field as: find $d_\theta \in \Theta_\mu$ such that

$$\int_{\Omega_\mu} \mathbf{K}_\mu \nabla d_\theta \cdot \nabla\hat{\tilde{\theta}}_\mu \, dV = 0, \quad \forall\hat{\tilde{\theta}}_\mu \in \Theta_\mu. \tag{25}$$

From the property of $\mathbf{K}_\mu$, clearly, this implies that

$$d_\theta = 0, \tag{26}$$

which is expected from the microscopic thermal analysis. From this, we obtain that $\tilde{\theta}_\mu$ solely depends on the macroscopic datum $\mathbf{g}$. That is, the macroscopic heat flux $\mathbf{q}$ is expressed in terms of the homogenized temperature gradient as

$$\mathbf{q} = -\mathbf{K}\mathbf{g}. \tag{27}$$

5 Multiscale Mechanical Analysis with Thermal Effects

5.1 Kinematical Admissibility

As in the previous section, we define in this case the macroscopic mechanical strain tensor $\boldsymbol{\varepsilon}$ at the point $\mathbf{x}$ of the macroscopic continuum, and link this strain to its microscopic counterpart $\boldsymbol{\varepsilon}_\mu$ defined over the domain of the RVE. The microscopic strain field $\boldsymbol{\varepsilon}_\mu$ is given by the symmetric part of the gradient of the microscopic displacement field $\mathbf{u}_\mu$. Then, the kinematical homogenization principle reads:

$$\boldsymbol{\varepsilon} := \frac{1}{V_\mu} \int_{\Omega_\mu} \nabla^s \mathbf{u}_\mu \, dV. \tag{28}$$

Taking into account the Green's formula in (28) we obtain the following equivalent expression for the homogenized (macroscopic) strain tensor $\boldsymbol{\varepsilon}$

$$\boldsymbol{\varepsilon} = \frac{1}{V_\mu} \int_{\partial\Omega_\mu} \mathbf{u}_\mu \otimes_s \mathbf{n} \, dS, \tag{29}$$

where, as before, $\mathbf{n}$ is the outward unit normal to the boundary $\partial\Omega_\mu$ and $\otimes_s$ denotes the symmetric tensor product of vectors. Note that, the above expression imposes a kinematical constraint over the admissible displacement fields over the RVE such that the kinematical homogenization principle (28) is satisfied. Now, without loss of generality, as done in the thermal case, it is possible split $\mathbf{u}_\mu$ into a sum of the macroscopic displacement field $\mathbf{u}$, the contribution provided by the macroscopic strain $\boldsymbol{\varepsilon}$ and a fluctuation displacement field $\tilde{\mathbf{u}}_\mu(\mathbf{y})$ (see Fig. 2)

$$\mathbf{u}_\mu(\mathbf{y}) = \mathbf{u} + \boldsymbol{\varepsilon}(\mathbf{y} - \mathbf{y}_o) + \tilde{\mathbf{u}}_\mu(\mathbf{y}). \tag{30}$$

With the above splitting, the microscopic strain field can be written as a sum

$$\nabla^s \mathbf{u}_\mu = \boldsymbol{\varepsilon} + \nabla^s \tilde{\mathbf{u}}_\mu, \tag{31}$$

of a homogeneous strain (uniform over the RVE) coinciding with the macroscopic strain and a field $\nabla^s \tilde{\mathbf{u}}_\mu$ corresponding to the contribution of the fluctuation of the microscopic strain around the homogenized (average) value. In order to remove rigid modes, and to proceed similarly to the thermal case seen in Sect. 4, we also assume the following constraint on the microscopic displacement field $\mathbf{u}_\mu$

$$\mathbf{u} = \frac{1}{V_\mu} \int_{\Omega_\mu} \mathbf{u}_\mu \, dV. \tag{32}$$

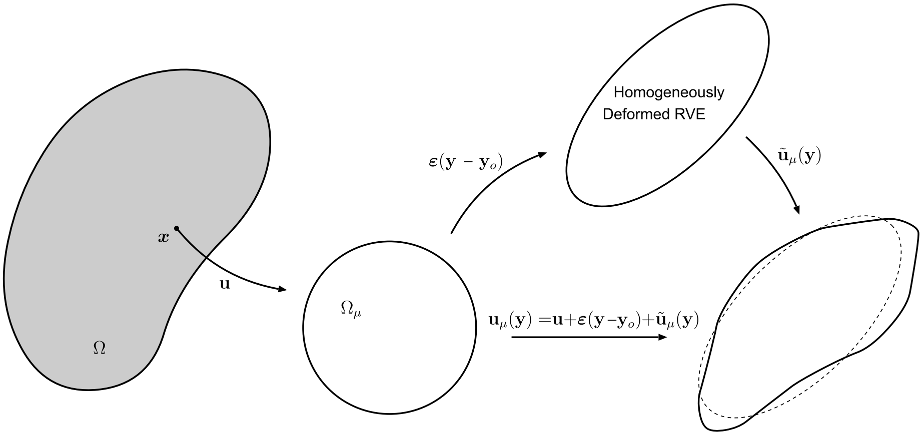

Fig. 2 Additive splitting of the microscopic displacement field

By introducing the additive splitting for the microscopic displacement field $\mathbf{u}_\mu$ into the above constraint, we obtain the following expression for the microscopic displacement fluctuation field

$$\int_{\Omega_\mu} \tilde{\mathbf{u}}_\mu \, dV = \mathbf{0}. \tag{33}$$

In this sense, the kinematical homogenization procedure introduced in (28) induces the minimally constrained space of admissible microscopic displacement fluctuation fields at the RVE

$$\boldsymbol{\mathcal{U}}_\mu := \left\{ \mathbf{u} \in \mathbf{H}^1(\Omega_\mu) : \int_{\Omega_\mu} \mathbf{u} \, dV = \mathbf{0}, \int_{\partial\Omega_\mu} \mathbf{u} \otimes_s \mathbf{n} \, dS = \mathbf{0} \right\}. \tag{34}$$

Hence, the space of kinematically admissible variations of the microscopic displacement field at the RVE is $\boldsymbol{\mathcal{U}}_\mu$ as well.

Remark 2 As in Remark 1, other multiscale models could be obtained by considering any other space of admissible functions, say $\boldsymbol{\mathcal{U}}_\mu^X$. It is just necessary that $\boldsymbol{\mathcal{U}}_\mu^X \subset \boldsymbol{\mathcal{U}}_\mu$. Examples of alternatives are the classical model with null boundary conditions or the one with periodic boundary conditions [6, 27].

5.2 The Hill–Mandel Principle and Its Variational Consequences

As in the thermal case, the physical bridging between macro and micro scales is provided by the *Hill–Mandel Principle of Macro-homogeneity* [16, 19], which is

$$\boldsymbol{\sigma} \cdot \hat{\boldsymbol{\varepsilon}} = \frac{1}{V_\mu} \int_{\Omega_\mu} \boldsymbol{\sigma}_\mu(\mathbf{u}_\mu, \theta_\mu) \cdot \nabla^s \hat{\mathbf{u}}_\mu \, dV, \quad \forall (\hat{\mathbf{u}}_\mu, \hat{\boldsymbol{\varepsilon}}) \text{ kinematically admissible.} \tag{35}$$

Introducing the decomposition (30) into (35), and recalling (8), leads to the following variational problem: given the macroscopic temperature θ, the macroscopic temperature gradient $\mathbf{g}$, the microscopic temperature fluctuation field $\tilde{\theta}_\mu$ (solution of (15)) and the macroscopic strain $\boldsymbol{\varepsilon}$, find $\boldsymbol{\sigma}$ and $\tilde{\mathbf{u}}_\mu \in \boldsymbol{\mathcal{U}}_\mu$ such that

$$\boldsymbol{\sigma} \cdot \hat{\boldsymbol{\varepsilon}} = \frac{1}{V_\mu} \int_{\Omega_\mu} \boldsymbol{\sigma}_\mu \big(\mathbf{u} + \boldsymbol{\varepsilon}(\mathbf{y} - \mathbf{y}_o) + \tilde{\mathbf{u}}_\mu, \theta + \mathbf{g} \cdot (\mathbf{y} - \mathbf{y}_o) + \tilde{\theta}_\mu\big) \cdot \big(\hat{\boldsymbol{\varepsilon}} + \nabla^s \hat{\tilde{\mathbf{u}}}_\mu\big)\, dV,$$
$$\forall \hat{\tilde{\mathbf{u}}}_\mu \in \boldsymbol{\mathcal{U}}_\mu \text{ and } \forall \hat{\boldsymbol{\varepsilon}}. \tag{36}$$

As before, using standard variational arguments, the Hill–Mandel principle provides two consequences: the microscopic mechanical equilibrium problem and the homogenization formula for the Cauchy stress.

Micro-mechanical equilibrium problem: Considering $\hat{\boldsymbol{\varepsilon}} = \mathbf{0}$ in (36) yields the microscopic mechanical equilibrium problem: given the macroscopic temperature θ, the macroscopic temperature gradient $\mathbf{g}$, the microscopic temperature fluctuation field $\tilde{\theta}_\mu$ (solution of (15)) and the macroscopic strain $\boldsymbol{\varepsilon}$, find the microscopic displacement fluctuation field $\tilde{\mathbf{u}}_\mu \in \boldsymbol{\mathcal{U}}_\mu$ such that

$$\int_{\Omega_\mu} \boldsymbol{\sigma}_\mu \big(\mathbf{u} + \boldsymbol{\varepsilon}(\mathbf{y} - \mathbf{y}_o) + \tilde{\mathbf{u}}_\mu, \theta + \mathbf{g} \cdot (\mathbf{y} - \mathbf{y}_o) + \tilde{\theta}_\mu\big) \cdot \nabla^s \hat{\tilde{\mathbf{u}}}_\mu\, dV = 0, \quad \forall \hat{\tilde{\mathbf{u}}}_\mu \in \boldsymbol{\mathcal{U}}_\mu. \tag{37}$$

Characterization of the macroscopic stress: Considering $\hat{\tilde{\mathbf{u}}}_\mu = \mathbf{0}$ in (36) results the characterization of the macroscopic stress state $\boldsymbol{\sigma}$: given the macroscopic temperature θ, its gradient $\mathbf{g}$, the field $\tilde{\theta}_\mu$ solution of problem (15), the macroscopic strain $\boldsymbol{\varepsilon}$, and $\tilde{\mathbf{u}}_\mu$—the solution of problem (37)—, compute $\boldsymbol{\sigma}$ as

$$\boldsymbol{\sigma} = \frac{1}{V_\mu} \int_{\Omega_\mu} \boldsymbol{\sigma}_\mu \big(\mathbf{u} + \boldsymbol{\varepsilon}(\mathbf{y} - \mathbf{y}_o) + \tilde{\mathbf{u}}_\mu, \theta + \mathbf{g} \cdot (\mathbf{y} - \mathbf{y}_o) + \tilde{\theta}_\mu\big)\, dV. \tag{38}$$

Notice that since the microscopic temperature field is being considered in the microscopic stress state, naturally, the formulation provides a macroscopic stress state which, in addition, depends upon the temperature gradient, which is an intrinsic feature of materials with microstructure. In Sect. 6 we will provide an account of the elements that are necessary to accommodate this material behavior in a thermodynamically consistent framework.

In this work, materials at the microscale follow the simplest constitutive thermoelastic model, which is

$$\boldsymbol{\sigma}_\mu(\mathbf{v}, \xi) = \mathbb{C}_\mu\big(\nabla^s \mathbf{v}\big) - \mathbf{B}_\mu \xi, \tag{39}$$

being $\mathbb{C}_\mu$ the fourth order elasticity tensor and $\mathbf{B}_\mu$ the second order thermomechanical expansion tensor. Assuming that the microstructural behavior of the materials is isotropic and homogeneous, we have

$$\begin{aligned} \mathbb{C}_\mu &= \frac{E_\mu}{1 - \nu_\mu^2}\big[(1 - \nu_\mu)\mathbb{I} + \nu_\mu(\mathbf{I} \otimes \mathbf{I})\big], \\ \mathbf{B}_\mu &= \frac{\alpha_\mu E_\mu}{1 - \nu_\mu^2}\big(1 + \nu_\mu(\mathrm{tr}\mathbf{I} - 1)\big)\mathbf{I}, \end{aligned} \tag{40}$$

with E_μ, ν_μ and α_μ denoting, respectively, the Young's modulus, the Poisson's ratio and the thermal expansion coefficient at the RVE. In (40) we use $\mathbf{I}$ and $\mathbb{I}$ to denote the second and fourth order identity tensors, respectively, while tr$(\cdot)$ is used to denote the trace operator applied to tensor $(\cdot)$.

Remark 3 Observe that the microscopic stress $\boldsymbol{\sigma}_\mu$ given in (39) is derived from a microscopic free energy function which is quadratic in the variables $(\nabla^s \mathbf{v}, \xi)$, that is

$$\psi_\mu(\nabla^s \mathbf{v}, \xi) = \frac{1}{2}\mathbb{C}_\mu(\nabla^s \mathbf{v}) \cdot (\nabla^s \mathbf{v}) - \mathbf{B}_\mu \cdot (\nabla^s \mathbf{v})\xi - \frac{1}{2} a_\mu \xi^2, \tag{41}$$

from which

$$\boldsymbol{\sigma}_\mu = \frac{\partial \psi_\mu}{\partial(\nabla^s \mathbf{v})} = \mathbb{C}_\mu(\nabla^s \mathbf{v}) - \mathbf{B}_\mu \xi, \tag{42}$$

while the microscopic entropy is given by

$$s_\mu = -\frac{\partial \psi_\mu}{\partial \xi} = a_\mu \xi + \mathbf{B}_\mu \cdot (\nabla^s \mathbf{v}). \tag{43}$$

At this point, we assume that all the material parameters involved in (41) are such that at the microscopic level the constitutive model holds convexity properties as in classical thermodynamics. In Sect. 6 we will expand the discussion about the bridging between the microscopic and the macroscopic thermodynamic settings.

Now we split the microscopic stress state using (8) and (30) as follows

$$\boldsymbol{\sigma}_\mu(\mathbf{u}_\mu, \theta_\mu) = \mathbb{C}_\mu \boldsymbol{\varepsilon} + \mathbb{C}_\mu(\nabla^s \tilde{\mathbf{u}}_\mu) - \mathbf{B}_\mu \theta - \mathbf{B}_\mu(\mathbf{g} \cdot (\mathbf{y} - \mathbf{y}_o)) - \mathbf{B}_\mu \tilde{\theta}_\mu, \tag{44}$$

and then, the closed form of the microscopic mechanical equilibrium problem reads: given $\boldsymbol{\varepsilon}$, θ, $\mathbf{g}$ and $\tilde{\theta}_\mu$, find $\tilde{\mathbf{u}}_\mu \in \boldsymbol{\mathcal{U}}_\mu$ such that

$$\begin{aligned} &\int_{\Omega_\mu} \mathbb{C}_\mu(\nabla^s \tilde{\mathbf{u}}_\mu) \cdot \nabla^s \hat{\tilde{\mathbf{u}}}_\mu \, dV \\ &\quad = -\int_{\Omega_\mu} \big(\mathbb{C}_\mu \boldsymbol{\varepsilon} - \mathbf{B}_\mu \theta - \mathbf{B}_\mu(\mathbf{g} \cdot (\mathbf{y} - \mathbf{y}_o)) - \mathbf{B}_\mu \tilde{\theta}_\mu\big) \cdot \nabla^s \hat{\tilde{\mathbf{u}}}_\mu \, dV, \quad \forall \hat{\tilde{\mathbf{u}}}_\mu \in \boldsymbol{\mathcal{U}}_\mu, \end{aligned} \tag{45}$$

and the corresponding homogenization formula for the macroscopic stress is

$$\begin{aligned} \boldsymbol{\sigma} &= \left(\frac{1}{V_\mu}\int_{\Omega_\mu} \mathbb{C}_\mu \, dV\right)\boldsymbol{\varepsilon} - \left(\frac{1}{V_\mu}\int_{\Omega_\mu} \mathbf{B}_\mu \, dV\right)\theta - \left(\frac{1}{V_\mu}\int_{\Omega_\mu} \mathbf{B}_\mu \otimes (\mathbf{y} - \mathbf{y}_o) \, dV\right)\mathbf{g} \\ &\quad + \frac{1}{V_\mu}\int_{\Omega_\mu} \mathbb{C}_\mu(\nabla^s \tilde{\mathbf{u}}_\mu) \, dV - \frac{1}{V_\mu}\int_{\Omega_\mu} \mathbf{B}_\mu \tilde{\theta}_\mu \, dV. \end{aligned} \tag{46}$$

5.3 The Homogenized Elastic and Thermal Expansion Tensors

In the constitutive multiscale model recently introduced, it has been presented how to use the macroscopic information (mechanical strain tensor $\boldsymbol{\varepsilon}$, temperature θ and temperature gradient $\mathbf{g}$) to obtain the microscopic temperature and displacement fields fully defined through the microscopic fluctuations of temperature and displacement, that is $\tilde{\theta}_\mu$ and $\tilde{\mathbf{u}}_\mu$, respectively. The basic idea now is to retrieve a closed form of the tangent macroscopic constitutive response from (46) in terms of the triple $(\boldsymbol{\varepsilon}, \theta, \mathbf{g})$. In the first place we compute the tangent problem from (45) with respect to the strain $\boldsymbol{\varepsilon}$. Proceeding analogously to the thermal case, we derive (45) with respect to $\boldsymbol{\varepsilon}$ and put $\mathbf{D}_{\boldsymbol{\varepsilon}} := \frac{\partial \tilde{\mathbf{u}}_\mu}{\partial \boldsymbol{\varepsilon}}$ (a third order tensor field), noting that $[\mathbf{D}_{\boldsymbol{\varepsilon}}]_{ij} = \frac{\partial \tilde{\mathbf{u}}_\mu}{\partial [\boldsymbol{\varepsilon}]_{ij}}$ (a vector field). This procedure leads us to the problem of finding $[\mathbf{D}_{\boldsymbol{\varepsilon}}]_{ij} \in \boldsymbol{\mathcal{U}}_\mu$ such that

$$\int_{\Omega_\mu} \mathbb{C}_\mu\big(\nabla^s[\mathbf{D}_{\boldsymbol{\varepsilon}}]_{ij}\big) \cdot \nabla^s \hat{\tilde{\mathbf{u}}}_\mu \, dV = -\int_{\Omega_\mu} \mathbb{C}_\mu(\mathbf{e}_i \otimes_s \mathbf{e}_j) \cdot \nabla^s \hat{\tilde{\mathbf{u}}}_\mu \, dV, \quad \forall \hat{\tilde{\mathbf{u}}}_\mu \in \boldsymbol{\mathcal{U}}_\mu, \tag{47}$$

for $i, j = 1, \dots, n$.

Thus, the macroscopic mechanical tangent operator is given by

$$\frac{\partial \boldsymbol{\sigma}}{\partial \boldsymbol{\varepsilon}} := \mathbb{C} = \overline{\mathbb{C}} + \widetilde{\mathbb{C}}, \tag{48}$$

where

$$\overline{\mathbb{C}} = \frac{1}{V_\mu} \int_{\Omega_\mu} \mathbb{C}_\mu \, dV, \tag{49}$$

and

$$\widetilde{\mathbb{C}} = \left[\frac{1}{V_\mu} \int_{\Omega_\mu} \big(\mathbb{C}_\mu\big(\nabla^s[\mathbf{D}_{\boldsymbol{\varepsilon}}]_{kl}\big)\big)_{ij} \, dV \right] (\mathbf{e}_i \otimes \mathbf{e}_j \otimes \mathbf{e}_k \otimes \mathbf{e}_l). \tag{50}$$

In the second place we compute the tangent problem from (45) with respect to the temperature θ. Using the same procedure, we derive (45) with respect to θ, call $\mathbf{d}_\theta := \frac{\partial \tilde{\mathbf{u}}_\mu}{\partial \theta}$ (a vector field) and recall that the microscopic temperature fluctuation field $\tilde{\theta}_\mu$ does not depend on the macroscopic temperature, according to (26). Therefore, we obtain the following problem: find $\mathbf{d}_\theta \in \boldsymbol{\mathcal{U}}_\mu$ such that

$$\int_{\Omega_\mu} \mathbb{C}_\mu\big(\nabla^s \mathbf{d}_\theta\big) \cdot \nabla^s \hat{\tilde{\mathbf{u}}}_\mu \, dV = \int_{\Omega_\mu} \mathbf{B}_\mu \cdot \nabla^s \hat{\tilde{\mathbf{u}}}_\mu \, dV, \quad \forall \hat{\tilde{\mathbf{u}}}_\mu \in \boldsymbol{\mathcal{U}}_\mu. \tag{51}$$

In this manner, the *first-order* thermal contribution to the macroscopic stress is governed by the following tensor

$$-\frac{\partial \boldsymbol{\sigma}}{\partial \theta} := \mathbf{B} = \overline{\mathbf{B}} + \widetilde{\mathbf{B}}, \tag{52}$$

where

$$\overline{\mathbf{B}} = \frac{1}{V_\mu} \int_{\Omega_\mu} \mathbf{B}_\mu \, dV, \tag{53}$$

and

$$\widetilde{\mathbf{B}} = -\frac{1}{V_\mu} \int_{\Omega_\mu} \mathbb{C}_\mu\big(\nabla^s \mathbf{d}_\theta\big) \, dV. \tag{54}$$

In an analogous way, we obtain the tangent problem of (45) with respect to the temperature gradient $\mathbf{g}$. By deriving (45) with respect to $\mathbf{g}$ and calling $\mathbf{D}_{\mathbf{g}} := \frac{\partial \tilde{\mathbf{u}}_\mu}{\partial \mathbf{g}}$ (a second order tensor field), which means $[\mathbf{D_g}]_i = \frac{\partial \tilde{\mathbf{u}}_\mu}{\partial [\mathbf{g}]_i}$ (a vector field), yields the variational problem for this tangent field: find $[\mathbf{D_g}]_i \in \mathcal{U}_\mu$ such that

$$\int_{\Omega_\mu} \mathbb{C}_\mu\big(\nabla^s[\mathbf{D_g}]_i\big)\cdot\nabla^s\hat{\tilde{\mathbf{u}}}_\mu\,dV = \int_{\Omega_\mu}\mathbf{B}_\mu\big([\mathbf{y}-\mathbf{y}_o]_i+[\mathbf{d_g}]_i\big)\cdot\nabla^s\hat{\tilde{\mathbf{u}}}_\mu\,dV,\quad \forall\hat{\tilde{\mathbf{u}}}_\mu\in\mathcal{U}_\mu, \tag{55}$$

for $i = 1,\ldots,n$. Above, recall that $\mathbf{d_g}$ expresses the sensitivity of the microscopic temperature fluctuation field $\tilde{\theta}_\mu$ with respect to the macroscopic temperature gradient $\mathbf{g}$, which is obtained by solving (21).

Hence, a *second-order* thermal contribution to the macroscopic stress state is given through the following tensor

$$-\frac{\partial\boldsymbol{\sigma}}{\partial\mathbf{g}} := \mathsf{G} = \overline{\mathsf{G}} + \widetilde{\mathsf{G}}, \tag{56}$$

where

$$\overline{\mathsf{G}} = \frac{1}{V_\mu}\int_{\Omega_\mu}\mathbf{B}_\mu\otimes(\mathbf{y}-\mathbf{y}_o)\,dV, \tag{57}$$

and

$$\widetilde{\mathsf{G}} = -\left[\frac{1}{V_\mu}\int_{\Omega_\mu}\big(\mathbb{C}_\mu\big(\nabla^s[\mathbf{D_g}]_k\big)\big)_{ij}\,dV - \frac{1}{V_\mu}\int_{\Omega_\mu}(\mathbf{B}_\mu)_{ij}[\mathbf{d_g}]_k\,dV\right](\mathbf{e}_i\otimes\mathbf{e}_j\otimes\mathbf{e}_k). \tag{58}$$

Finally, the macroscopic stress $\boldsymbol{\sigma}$ can be written in terms of the above homogenized quantities as

$$\boldsymbol{\sigma} = \mathbb{C}\boldsymbol{\varepsilon} - \mathbf{B}\theta - \mathsf{G}\mathbf{g}. \tag{59}$$

Here, the tensor G represents explicitly the constitutive property responsible for the stress generation at macroscopic level due to the gradient of the temperature field at the same level.

6 Multiscale Thermodynamic Setting

As commented in Remark 3, the microscopic thermodynamics is the classical one, in the sense of the relation between internal energy and entropy, which leads to the classical Clausius–Duhem inequality. Being e_μ, s_μ and ψ_μ the microscopic internal energy, microscopic entropy and microscopic free energy function, respectively, this implies that these quantities are related through

$$e_\mu = s_\mu\theta_\mu + \psi_\mu(\theta_\mu,\boldsymbol{\varepsilon}_\mu), \tag{60}$$

with s_μ and θ_μ being dual variables in the sense of the Legendre transform. Then we have

$$s_\mu = -\frac{\partial\psi_\mu}{\partial\theta_\mu}\quad\text{and}\quad\theta_\mu = \frac{\partial e_\mu}{\partial s_\mu}. \tag{61}$$

Nevertheless, the existence of a macroscopic temperature gradient $\mathbf{g}$ poses the problem of considering microscopic temperature fields θ_μ which make the macroscopic stress state $\boldsymbol{\sigma}$ sensitive to this temperature gradient $\mathbf{g}$. In a classical thermodynamic setting it is well known that $\boldsymbol{\sigma}$ cannot depend on $\mathbf{g}$. Hence, the aim of this section is to provide the extended macroscopic thermodynamic context in which the multiscale constitutive model developed in Sects. 4 and 5 has to be considered.

The theoretical foundations employed here are based on the developments presented in [24, 25]. For a thorough discussion of the underlying elements in this framework the reader is referred to [25]. The basic modification to the classical thermodynamics foundations is introduced by writing the macroscopic internal energy as follows

$$e = s\theta + \mathbf{r}\cdot\mathbf{g} + \psi(\theta, \mathbf{g}, \boldsymbol{\varepsilon}), \tag{62}$$

where, now, $(s, \mathbf{r})$ and $(\theta, \mathbf{g})$ are dual pairs in the sense of the Legendre transform. Analogously, it is possible to obtain the following relations

$$\begin{aligned} s &= -\frac{\partial \psi}{\partial \theta}, \qquad & \mathbf{r} &= -\frac{\partial \psi}{\partial \mathbf{g}}, \\ \theta &= \frac{\partial e}{\partial s} \quad \text{and} \quad & \mathbf{g} &= \frac{\partial e}{\partial \mathbf{r}}. \end{aligned} \tag{63}$$

With these considerations, the functional form $\psi(\theta, \mathbf{g}, \boldsymbol{\varepsilon})$ is allowed.

Indeed, in the multiscale context consider that

$$\psi = \frac{1}{V_\mu}\int_{\Omega_\mu} \psi_\mu \, dV. \tag{64}$$

The macroscopic entropy is given by deriving with respect to θ, that is

$$s = -\frac{\partial \psi}{\partial \theta} = -\frac{1}{V_\mu}\int_{\Omega_\mu} \frac{\partial \psi_\mu}{\partial \theta}\, dV = -\frac{1}{V_\mu}\int_{\Omega_\mu} \frac{\partial \psi_\mu}{\partial \theta_\mu}\, dV = \frac{1}{V_\mu}\int_{\Omega_\mu} s_\mu \, dV, \tag{65}$$

where we have used the fact that $\frac{\partial \theta_\mu}{\partial \theta} = 1$ in view of (26). In turn, we have

$$\begin{aligned} \mathbf{r} = -\frac{\partial \psi}{\partial \mathbf{g}} &= -\frac{1}{V_\mu}\int_{\Omega_\mu} \frac{\partial \psi_\mu}{\partial \mathbf{g}}\, dV \\ &= -\frac{1}{V_\mu}\int_{\Omega_\mu} \frac{\partial \psi_\mu}{\partial \theta_\mu}(\mathbf{y} - \mathbf{y}_o + \mathbf{d}_\mathbf{g})\, dV = \frac{1}{V_\mu}\int_{\Omega_\mu} s_\mu (\mathbf{y} - \mathbf{y}_o + \mathbf{d}_\mathbf{g})\, dV, \end{aligned} \tag{66}$$

for which we have taken into account that $\frac{\partial \theta_\mu}{\partial \mathbf{g}} = \mathbf{y} - \mathbf{y}_o + \mathbf{d}_\mathbf{g}$, which stems from $\theta_\mu = \theta + \mathbf{g}\cdot(\mathbf{y} - \mathbf{y}_o) + \mathbf{g}\cdot\mathbf{d}_\mathbf{g}$. Then, we observe that

$$\begin{aligned} \frac{1}{V_\mu}\int_{\Omega_\mu} e_\mu \, dV &= \frac{1}{V_\mu}\int_{\Omega_\mu} (s_\mu\theta_\mu + \psi_\mu)\, dV \\ &= \frac{1}{V_\mu}\int_{\Omega_\mu} \big(s_\mu\big(\theta + \mathbf{g}\cdot(\mathbf{y} - \mathbf{y}_o) + \tilde{\theta}_\mu\big) + \psi_\mu\big)\, dV \\ &= \frac{1}{V_\mu}\int_{\Omega_\mu} s_\mu\theta \, dV + \frac{1}{V_\mu}\int_{\Omega_\mu} s_\mu\big(\mathbf{g}\cdot(\mathbf{y} - \mathbf{y}_o) + \mathbf{g}\cdot\mathbf{d}_\mathbf{g}\big)\, dV + \frac{1}{V_\mu}\int_{\Omega_\mu} \psi_\mu \, dV \\ &= s\theta + \mathbf{r}\cdot\mathbf{g} + \psi = e. \end{aligned} \tag{67}$$

With this extended macroscopic thermodynamics it can be shown (see [25]) that the macroscopic steady state equation for the energy balance remains the classical one. The impact of the introduction of $\mathbf{r}$, called the entropy vector, and the dependence of ψ with respect to $\mathbf{g}$ is manifested in the transient problem, which in turn gives rise to governing equations that allow thermal waves to occur [24, 39]. This is consistent with the foundations of the extended thermodynamics as presented in [22].

Making use of this extended thermodynamics at the macroscopic scale is necessary in order to accommodate the natural dependence of the stress state with respect to the temperature gradient when employing this class of multiscale thermomechanical constitutive modeling. The multiscale constitutive model constructed this way is consistent in the sense that the temperature fluctuations that arise at the microscopic problem when performing the multiscale thermal analysis are equally considered in the multiscale mechanical analysis with thermal effects. Clearly, this is one of the fundamental objectives of a multiscale theory, that is, to use simple microscopic relations in order to retrieve complex macroscopic material behavior.

Remark 4 Regarding the convexity of the macroscopic model let us look into the convexity of $-\psi$ with respect to the variables θ and $\mathbf{g}$, as in [24, 25]. Firstly, for the temperature we have that

$$\begin{aligned} -\frac{\partial^2\psi}{\partial\theta^2} &= -\frac{1}{V_\mu}\int_{\Omega_\mu}\frac{\partial^2\psi_\mu}{\partial\theta^2}\,dV \\ &= -\frac{1}{V_\mu}\int_{\Omega_\mu}\frac{\partial^2\psi_\mu}{\partial\theta_\mu^2}\,dV = \frac{1}{V_\mu}\int_{\Omega_\mu} a_\mu\,dV. \end{aligned} \tag{68}$$

Then, if $a_\mu > 0$ it turns out that $-\frac{\partial^2\psi}{\partial\theta^2} > 0$. In addition, for the temperature gradient, it results

$$\begin{aligned} -\frac{\partial^2\psi}{\partial\mathbf{g}^2} &= -\frac{1}{V_\mu}\int_{\Omega_\mu}\frac{\partial^2\psi_\mu}{\partial\mathbf{g}^2}\,dV \\ &= -\frac{1}{V_\mu}\int_{\Omega_\mu}\frac{\partial^2\psi_\mu}{\partial\theta_\mu^2}\big[(\mathbf{y}-\mathbf{y}_o+\mathbf{d}_\mathbf{g})\otimes(\mathbf{y}-\mathbf{y}_o+\mathbf{d}_\mathbf{g})\big]\,dV \\ &= \frac{1}{V_\mu}\int_{\Omega_\mu} a_\mu\big[(\mathbf{y}-\mathbf{y}_o+\mathbf{d}_\mathbf{g})\otimes(\mathbf{y}-\mathbf{y}_o+\mathbf{d}_\mathbf{g})\big]\,dV. \end{aligned} \tag{69}$$

Then, if $a_\mu > 0$ we have that $-\frac{\partial^2\psi}{\partial\mathbf{g}^2}$ is a positive definite second order tensor. Therefore, we conclude that the convexity of the model follows from the convexity of the constitutive model at the microstructure.

7 Concluding Remarks

In this work a general variational formulation for multiscale constitutive models in the thermomechanical setting has been presented. The multiscale analysis was based on the volume averaging concept over a local representative volume element (RVE) and the Hill–Mandel Principle of Macro-homogeneity for the scale transition. The contribution of the present work has been the consistent formulation of the multiscale constitutive model in the thermomechanical setting taking into account the microscopic temperature fluctuations within the micro-mechanical problem. Even making use of classical thermodynamics and material behavior at the microscopic level, it has been shown that this approach yields a macroscopic material behavior in which the stress state depends upon the temperature gradient. This is possible in view of having considered an extended thermodynamics ruling at the macroscopic level, whose ingredients are related to the microscopic scale in a fully closed form.

The coupling term at macroscopic level between the mechanical stress and the temperature gradient arises in several engineering applications. To illustrate this fact, one application where this term can be of paramount importance is in the solidification and phase transition of metal-based materials. During the early stage of the solidification (liquid state), the cooling rate is the most important property that governs the microstructure evolution. This means that different microstructures may evolve from the same base materials if we change the cooling rate during this stage. However, when the base material became solid, residual stresses appear as consequence of the cooling phenomena. During this stage, thermal stresses are induced because of the thermal expansion constitutive properties. In the same way, if some part of the piece has higher temperatures than another, during the cooling phenomena, gradients of temperature occur, which are also responsible for this residual stress. These residual stresses are very important in the manufacture industry because they are responsible for the damage initialization and initial geometrical distortions in the pieces made by metal materials, among others.

In order to summarize the obtained results, in the following boxes we presents the ingredients of the model developed here

Box 1: Multiscale Thermal Model

(1a) Micro-thermal equilibrium problem: given $\mathbf{g}$, find $\tilde{\theta}_\mu \in \Theta_\mu$ such that

$$\int_{\Omega_\mu} \mathbf{K}_\mu \nabla\tilde{\theta}_\mu \cdot \nabla\hat{\tilde{\theta}}_\mu \, dV = -\int_{\Omega_\mu} \mathbf{K}_\mu \mathbf{g} \cdot \nabla\hat{\tilde{\theta}}_\mu \, dV, \quad \forall \hat{\tilde{\theta}}_\mu \in \Theta_\mu,$$

where

$$\Theta_\mu := \left\{ v \in H^1(\Omega_\mu) : \int_{\Omega_\mu} v \, dV = 0, \int_{\partial\Omega_\mu} v\mathbf{n} \, dS = 0 \right\}.$$

(1b) Macroscopic heat flux

$$\mathbf{q} = -\left(\frac{1}{V_\mu}\int_{\Omega_\mu} \mathbf{K}_\mu \, dV\right)\mathbf{g} - \frac{1}{V_\mu}\int_{\Omega_\mu} \mathbf{K}_\mu \nabla\tilde{\theta}_\mu \, dV.$$

(1c) Macroscopic thermal tangent operator

$$-\frac{\partial \mathbf{q}}{\partial \mathbf{g}} := \mathbf{K} = \overline{\mathbf{K}} + \widetilde{\mathbf{K}},$$

where

$$\overline{\mathbf{K}} = \frac{1}{V_\mu}\int_{\Omega_\mu} \mathbf{K}_\mu \, dV \quad \text{and} \quad \widetilde{\mathbf{K}} = \left[\frac{1}{V_\mu}\int_{\Omega_\mu} \left(\mathbf{K}_\mu \nabla[\mathbf{d_g}]_j\right)_i dV\right](\mathbf{e}_i \otimes \mathbf{e}_j),$$

being $[\mathbf{d_g}]_i$ the solutions of the set of variational equations: find $[\mathbf{d_g}]_i \in \Theta_\mu$, such that

$$\int_{\Omega_\mu} \mathbf{K}_\mu \nabla[\mathbf{d_g}]_i \cdot \nabla\hat{\tilde{\theta}}_\mu \, dV = -\int_{\Omega_\mu} \mathbf{K}_\mu \mathbf{e}_i \cdot \nabla\hat{\tilde{\theta}}_\mu \, dV, \quad \forall \hat{\tilde{\theta}}_\mu \in \Theta_\mu,$$

for $i = 1, \ldots, n$.

Box 2: Multiscale Mechanical Model with Thermal Effects

(2a) Micro-mechanical equilibrium problem: given $\boldsymbol{\varepsilon}$, θ, $\mathbf{g}$ and $\tilde{\theta}_\mu$, find $\tilde{\mathbf{u}}_\mu \in \mathcal{U}_\mu$ such that

$$\int_{\Omega_\mu} \mathbb{C}_\mu(\nabla^s \tilde{\mathbf{u}}_\mu) \cdot \nabla^s \hat{\tilde{\mathbf{u}}}_\mu \, dV$$

$$= -\int_{\Omega_\mu} (\mathbb{C}_\mu \boldsymbol{\varepsilon} - \mathbf{B}_\mu \theta - \mathbf{B}_\mu(\mathbf{g} \cdot (\mathbf{y} - \mathbf{y}_o)) - \mathbf{B}_\mu \tilde{\theta}_\mu) \cdot \nabla^s \hat{\tilde{\mathbf{u}}}_\mu \, dV, \quad \forall \hat{\tilde{\mathbf{u}}}_\mu \in \mathcal{U}_\mu, \quad \text{where}$$

$$\mathcal{U}_\mu := \left\{ \mathbf{v} \in \mathbf{H}^1(\Omega_\mu) : \int_{\Omega_\mu} \mathbf{v} \, dV = 0, \int_{\partial\Omega_\mu} \mathbf{v} \otimes_s \mathbf{n} \, dS = 0 \right\}.$$

(2b) Macroscopic stress

$$\boldsymbol{\sigma} = \left(\frac{1}{V_\mu} \int_{\Omega_\mu} \mathbb{C}_\mu \, dV \right) \boldsymbol{\varepsilon} - \left(\frac{1}{V_\mu} \int_{\Omega_\mu} \mathbf{B}_\mu \, dV \right) \theta - \left(\frac{1}{V_\mu} \int_{\Omega_\mu} \mathbf{B}_\mu \otimes (\mathbf{y} - \mathbf{y}_o) \, dV \right) \mathbf{g}$$

$$+ \frac{1}{V_\mu} \int_{\Omega_\mu} \mathbb{C}_\mu(\nabla^s \tilde{\mathbf{u}}_\mu) \, dV - \frac{1}{V_\mu} \int_{\Omega_\mu} \mathbf{B}_\mu \tilde{\theta}_\mu \, dV.$$

(2ci) Macroscopic mechanical tangent operator

$$\frac{\partial \boldsymbol{\sigma}}{\partial \boldsymbol{\varepsilon}} := \mathbb{C} = \overline{\mathbb{C}} + \widetilde{\mathbb{C}}, \quad \text{where}$$

$$\overline{\mathbb{C}} = \frac{1}{V_\mu} \int_{\Omega_\mu} \mathbb{C}_\mu \, dV \quad \text{and} \quad \widetilde{\mathbb{C}} = \left[\frac{1}{V_\mu} \int_{\Omega_\mu} (\mathbb{C}_\mu(\nabla^s [\mathbf{D}_{\boldsymbol{\varepsilon}}]_{kl}))_{ij} \, dV \right] (\mathbf{e}_i \otimes \mathbf{e}_j \otimes \mathbf{e}_k \otimes \mathbf{e}_l),$$

being $[\mathbf{D}_{\boldsymbol{\varepsilon}}]_{ij}$ the solutions of the set of variational equations: find $[\mathbf{D}_{\boldsymbol{\varepsilon}}]_{ij} \in \mathcal{U}_\mu$, such that

$$\int_{\Omega_\mu} \mathbb{C}_\mu(\nabla^s [\mathbf{D}_{\boldsymbol{\varepsilon}}]_{ij}) \cdot \nabla^s \hat{\tilde{\mathbf{u}}}_\mu \, dV = -\int_{\Omega_\mu} \mathbb{C}_\mu(\mathbf{e}_i \otimes_s \mathbf{e}_j) \cdot \nabla^s \hat{\tilde{\mathbf{u}}}_\mu \, dV, \quad \forall \hat{\tilde{\mathbf{u}}}_\mu \in \mathcal{U}_\mu,$$

for $i, j = 1, \ldots, n$.

(2cii) Macroscopic first-order thermal tangent operator

$$-\frac{\partial \boldsymbol{\sigma}}{\partial \theta} := \mathbf{B} = \overline{\mathbf{B}} + \widetilde{\mathbf{B}}, \quad \text{where}$$

$$\overline{\mathbf{B}} = \frac{1}{V_\mu} \int_{\Omega_\mu} \mathbf{B}_\mu \, dV \quad \text{and} \quad \widetilde{\mathbf{B}} = -\frac{1}{V_\mu} \int_{\Omega_\mu} \mathbb{C}_\mu(\nabla^s \mathbf{d}_\theta) \, dV,$$

being $\mathbf{d}_\theta$ the solution of the variational problem: find $\mathbf{d}_\theta \in \mathcal{U}_\mu$ such that

$$\int_{\Omega_\mu} \mathbb{C}_\mu(\nabla^s \mathbf{d}_\theta) \cdot \nabla^s \hat{\tilde{\mathbf{u}}}_\mu \, dV = \int_{\Omega_\mu} \mathbf{B}_\mu \cdot \nabla^s \hat{\tilde{\mathbf{u}}}_\mu \, dV, \quad \forall \hat{\tilde{\mathbf{u}}}_\mu \in \mathcal{U}_\mu.$$

(2ciii) Macroscopic second-order thermal tangent operator

$$-\frac{\partial \boldsymbol{\sigma}}{\partial \mathbf{g}} := \mathbf{G} = \overline{\mathbf{G}} + \widetilde{\mathbf{G}}, \quad \text{where}$$

$$\overline{\mathbf{G}} = \frac{1}{V_\mu} \int_{\Omega_\mu} \mathbf{B}_\mu \otimes (\mathbf{y} - \mathbf{y}_o) \, dV, \quad \text{and}$$

$$\widetilde{\mathbf{G}} = -\left[\frac{1}{V_\mu} \int_{\Omega_\mu} (\mathbb{C}_\mu(\nabla^s [\mathbf{D}_\mathbf{g}]_k))_{ij} \, dV - \frac{1}{V_\mu} \int_{\Omega_\mu} (\mathbf{B}_\mu)_{ij} [\mathbf{d}_\mathbf{g}]_k \, dV \right] (\mathbf{e}_i \otimes \mathbf{e}_j \otimes \mathbf{e}_k).$$

Being $[\mathbf{D}_\mathbf{g}]_i$ the solutions of the variational problem: find $[\mathbf{D}_\mathbf{g}]_i \in \mathcal{U}_\mu$ such that

$$\int_{\Omega_\mu} \mathbb{C}_\mu(\nabla^s [\mathbf{D}_\mathbf{g}]_i) \cdot \nabla^s \hat{\tilde{\mathbf{u}}}_\mu \, dV = \int_{\Omega_\mu} \mathbf{B}_\mu([\mathbf{y} - \mathbf{y}_o]_i + [\mathbf{d}_\mathbf{g}]_i) \cdot \nabla^s \hat{\tilde{\mathbf{u}}}_\mu \, dV, \quad \forall \hat{\tilde{\mathbf{u}}}_\mu \in \mathcal{U}_\mu,$$

for $i = 1, \ldots, n$.

Box 3: Multiscale Thermodynamic Setting

(3a) Microscopic free energy function

$$e_\mu = s_\mu \theta_\mu + \psi_\mu(\theta_\mu, \boldsymbol{\varepsilon}_\mu),$$

with

$$s_\mu = -\frac{\partial \psi_\mu}{\partial \theta_\mu} \quad \text{and} \quad \theta_\mu = \frac{\partial e_\mu}{\partial s_\mu}.$$

(3b) Macroscopic free energy function

$$e = s\theta + \mathbf{r} \cdot \mathbf{g} + \psi(\theta, \mathbf{g}, \boldsymbol{\varepsilon}),$$

with

$$s = -\frac{\partial \psi}{\partial \theta} = \frac{1}{V_\mu} \int_{\Omega_\mu} s_\mu \, dV, \qquad \mathbf{r} = -\frac{\partial \psi}{\partial \mathbf{g}} = \frac{1}{V_\mu} \int_{\Omega_\mu} s_\mu (\mathbf{y} - \mathbf{y}_o + \mathbf{d}_\mathbf{g}) \, dV,$$

$$\theta = \frac{\partial e}{\partial s} \quad \text{and} \quad \mathbf{g} = \frac{\partial e}{\partial \mathbf{r}}.$$

Almost as a corollary, it has been shown that there are just two basic ingredients in this class of multiscale models: (i) the homogenization principles (temperature, temperature gradient and strain in the present problem) and (ii) the Hill–Mandel—variational—Principle of Macro-homogeneity. From these two pillars, the characterization of dual variables (heat flux and stress in the present problem), microscopic thermal and mechanical equilibrium problems and tangent operators arise as a consequence of the virtual power principle bridging the two scales.

Acknowledgements This research was partly supported by ANPCyT (National Agency for Scientific and Technical Promotion) and PID-UTN (Research and Development Program of the National Technological University) of Argentina, under grants N° PICT 2010-1259 and PID/IFN 1417, respectively. Also, we received support of the CNPq (Brazilian Research Council) and FAPERJ (Research Foundation of the State of Rio de Janeiro) agencies of Brazil. The support of all these agencies is gratefully acknowledged.

References

1. Bensoussan, A., Lions, J.L., Papanicolau, G.: Asymptotic Analysis for Periodic Microstructures. North Holland, Amsterdam (1978)
2. Bitsadze, L., Jaiani, G.: Some basic boundary value problems of the plane thermoelasticity with microtemperatures. Math. Methods Appl. Sci. (2012). doi:10.1002/mma.2652
3. Boutin, C.: Microstructural influence on heat conduction. Int. J. Heat Mass Transf. **38**, 3181–3195 (1995)
4. Cardona, J.-M., Forest, S., Sievert, R.: Towards a theory of second grade thermoelasticity. Extr. Math. **14**, 127–140 (1999)
5. Chen, H., Liu, Y., Zhao, X., Lanir, Y., Kassab, G.S.: A micromechanics finite-strain constitutive model of fibrous tissue. J. Mech. Phys. Solids **59**, 1823–1837 (2011)
6. de Souza Neto, E.A., Feijóo, R.A.: Variational foundations of large strain multiscale solid constitutive models: kinematical formulation. In: Advanced Computational Materials Modeling: From Classical to Multi-Scale Techniques. Wiley-VCH, Weinheim (2011)
7. Ene, H.I.: On linear thermoelasticity of composite materials. Int. J. Eng. Sci. **21**(5), 443–448 (1983)
8. Forest, S., Aifantis, E.C.: Some links between recent gradient thermo-elasto-plasticity theories and the thermomechanics of generalized continua. Int. J. Solids Struct. **47**, 3367–3376 (2010)
9. Forest, S., Amestoy, M.: Hypertemperature in thermoelastic solids. C. R., Méc. **336**(4), 347–353 (2008)
10. Forest, S., Cardona, J.-M., Sievert, R.: Thermoelasticity of Second-Grade Continua. Continuum Thermomechanics: The Art and Science of Modelling Material Behaviour, Paul Germain's Anniversary Volume. Kluwer Academic, Norwell (2000)

11. Francfort, G.A.: Homogenization and linear thermoelasticity. SIAM J. Math. Anal. **14**(4), 696–708 (1983)
12. Francfort, G.A., Suquet, P.M.: Homogenization and mechanical dissipation in thermoviscoelasticity. Arch. Ration. Mech. Anal. **96**(3), 265–293 (1986)
13. Germain, P., Nguyen, Q.S., Suquet, P.: Continuum thermodynamics. J. Appl. Mech. **50**(4), 1010–1020 (1983)
14. Giusti, S.M., Novotny, A.A., de Souza Neto, E.A., Feijóo, R.A.: Sensitivity of the macroscopic thermal conductivity tensor to topological microstructural changes. Comput. Methods Appl. Mech. Eng. **198**(5–8), 727–739 (2009)
15. Grot, R.A.: Thermodynamics of a continuum with microstructure. Int. J. Eng. Sci. **7**, 801–814 (1969)
16. Hill, R.: A self-consistent mechanics of composite materials. J. Mech. Phys. Solids **13**(4), 213–222 (1965)
17. Ireman, P., Nguyen, Q.-S.: Using the gradients of temperature and internal parameters in continuum thermodynamics. C. R., Méc. **332**(4), 249–255 (2004)
18. Khisaeva, Z.F., Ostoja-Starzewski, M.: On the size of RVE in finite elasticity of random composites. J. Elast. **85**(2), 153–173 (2006)
19. Mandel, J.: Plasticité Classique et Viscoplasticité. CISM Lecture Notes. Springer, Udine (1971)
20. Michel, J.C., Moulinec, H., Suquet, P.: Effective properties of composite materials with periodic microstructure: a computational approach. Comput. Methods Appl. Mech. Eng. **172**(1–4), 109–143 (1999)
21. Miehe, C., Schotte, J., Schröder, J.: Computational micro-macro transitions and overall moduli in the analysis of polycrystals at large strains. Comput. Mater. Sci. **16**(1–4), 372–382 (1999)
22. Müller, I.M., Ruggeri, T.: Rational Extended Thermodynamics. Tracts in Natural Philosophy, vol. 37. Springer, Berlin (1998)
23. Neff, P., Forest, S.: A geometrically exact micromorphic model for elastic metallic foams accounting for affine microstructure. Modelling, existence of minimizers, identification of moduli and computational results. J. Elast. **87**(2–3), 239–276 (2007)
24. Nguyen, Q.-S.: On standard dissipative gradient models. Ann. Solid Struct. Mech. **1**, 79–86 (2010)
25. Nguyen, Q.-S., Andrieux, S.: The non-local generalized standard approach: a consistent gradient theory. C. R., Méc. **333**(2), 139–145 (2005)
26. Özdemir, I., Brekelmans, W., Geers, M.: Computational homogenization for heat conduction in heterogeneous solids. Int. J. Numer. Methods Eng. **73**(2), 185–204 (2008)
27. Peric, D., de Souza Neto, E.A., Feijóo, R.A., Partovi, M., Carneiro Molina, A.J.: On micro-to-macro transitions for multi-scale analysis of non-linear heterogeneous materials: unified variational basis and finite element implementation. Int. J. Numer. Methods Eng. **87**, 149–170 (2011)
28. Riha, P.: On the microcontinuum model of heat conduction in materials with inner structure. Int. J. Eng. Sci. **14**, 529–535 (1976)
29. Ieşan, D.: On the theory of heat conduction in micromorphic continua. Int. J. Eng. Sci. **40**, 1859–1878 (2002)
30. Ieşan, D.: On a theory of thermoviscoelastic materials with voids. J. Elast. **104**(1–2), 369–384 (2011)
31. Ieşan, D., Nappa, L.: On the theory of heat for micromorphic bodies. Int. J. Eng. Sci. **43**, 17–32 (2005)
32. Ieşan, D., Quintanilla, R.: On thermoelastic bodies with inner structure and microtemperatures. Aust. J. Math. Anal. Appl. **354**, 12–23 (2009)
33. Sanchez-Palencia, E.: Non-homogeneous Media and Vibration Theory. Lecture Notes in Physics, vol. 127. Springer, Berlin (1980)
34. Sanchez-Palencia, E.: Homogenization method for the study of composite media. In: Asymptotic Analysis. II. Surveys and New Trends. Lecture Notes in Mathematics, vol. 985, pp. 192–214. Springer, Berlin (1983)
35. Speirs, D.C.D., de Souza Neto, E.A., Perić, D.: An approach to the mechanical constitutive modelling of arterial tissue based on homogenization and optimization. J. Biomech. **41**(12), 2673–2680 (2008)
36. Temizer, I., Wriggers, P.: Homogenization in finite thermoelasticity. J. Mech. Phys. Solids **59**, 344–372 (2011)
37. Terada, K., Kurumatani, M., Ushida, T., Kikuchi, N.: A method of two-scale thermo-mechanical analysis for porous solids with micro-scale heat transfer. Comput. Mech. **46**(2), 269–285 (2010)
38. Özdemir, I., Brekelmans, W.A.M., Geers, M.G.D.: FE^2 computational homogenization for the thermo-mechanical analysis of heterogeneous solids. Comput. Methods Appl. Mech. Eng. **198**, 602–613 (2008)
39. Özisik, M.N., Tzou, D.Y.: On the wave theory in heat conduction. J. Heat Transfer **116**, 526–535 (1994)