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EFFECTIVE PROPERTIES OF DISSIPATIVE COMPOSITES UNDER FULLY COUPLED THERMOMECHANICAL PROCESSES

1

George Chatzigeorgiou¹, Nicolas Charalambakis², Yves Chemisky¹, Fodil Meraghni¹

¹LEM3-UMR 7239 CNRS, ENSAM, 4 rue Augustin Fresnel, 57078 Metz, France Emails: georges.chatzigeorgiou@ensam.eu, yves.chemisky@ensam.eu, fodil.meraghni@ensam.eu

²Department of Civil Engineering, Aristotle University of Thessaloniki, 54124 Thessaloniki, Greece Email: charalam@civil.auth.gr

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Abstract

The current work deals with periodic composite media undergoing fully coupled thermomechanical loading. In these composites the material constituents are considered to obey the generalized standard materials laws. The aim of this research is to provide a proper homogenization framework that describes accurately all set of equations in both microscopic and macroscopic levels. The main tool of the study is the asymptotic expansion homogenization technique, which permits to deduce useful results about the energy potentials and constitutive laws that characterize the material response in both scales. In order to overcome the difficulty that the internal dissipation in the macroscale cannot be split analytically in terms of thermodynamic forces and fluxes, an incremental, linearized formulation is proposed. This formulation allows to identify proper thermomechanical tangent moduli for the macroscale problem and thus design an implicit computational scheme. The capability of this framework is illustrated with a numerical example on multilayered composites undergoing viscoplastic mechanisms.

1. Introduction

Nowadays composite materials are utilized in a vast variety of engineering applications. The automotive and aerospace industry have an increased need for smart and multifunctional materials able to be adapted in structures with high demands in strength, durability, and at the same time to have long lifetime. In many occasions the composite materials operate at stress levels where dissipative phenomena occur, like viscoelasticity, viscoplasticity etc. These mechanisms are often accompanied by significant temperature variations, affecting in return the material behavior.

Models with strong thermomechanical couplings have been already included in the study of homogeneous media through the framework of the generalized standard materials [1]. However, in the case of composite materials, very few works have been devoted to identify the fully coupled thermomechanical behavior of composites. This topic is nowadays of a great importance since, for instance, fatigue of composites is a complicated mechanism that depends not only on the stress state, but also on the energy dissipation that occurs during inelastic mechanisms. Thus, an appropriate study of the fatigue of a structure requires to consider the energy exchanges during thermomechanical loading cycles.

The asymptotic expansion homogenization (AEH) method, originally developed in the late seventies [2], is a homogenization framework that permits to study media with periodic microstructure. This methodology has been implemented successfully in thermoelastic composites, as well as in composites

with plastic mechanisms [3]. Most of the composite studies in the literature focus exclusively on the mechanical response. A limited number of works combine the conservations of linear momentum and energy in fully coupled nonlinear thermomechanical processes [4, 5].

This contribution is based on a recent work of the authors [6]. It presents a systematic study of the homogenization of periodic composites under fully coupled thermomechanical loading conditions, considering small deformation processes. The advantage of the proposed approach is that it is very general, without considering apriori a specific type of constitutive law or inelastic behavior for the various constituents of the composite. The developed framework i) identifies the micro and macro conservation laws and ii) investigates how a general energy potential is properly formulated in both scales. This study proves with a systematic and consistent manner which variables and equations can be rigorously identified in the macroscopic scale and which variables require either additional hypotheses or numerical treatment (as it is suggested here with the linearized incremental formulation).

2. Asymptotic expansion homogenization framework

The asymptotic expansion homogenization (AEH) approach is a framework that treats a composite material as a two scales mathematical problem. The first scale, the microscopic, takes into account the microstructure (material constituents, geometric characteristics). The second scale, the macroscopic, describes the response of the overall body as if it is a hypothetical homogeneous medium. The scope of AEH is to identify the connection between the scales in terms of: a) the various thermomechanical fields and b) the conservation laws and the constitutive relations that dictate the material response.

At the macroscale, the overall body occupies the space $\bar{\mathcal{D}}$, which is bounded by a surface $\partial \bar{\mathcal{D}}$ with unit vector \bar{n}_i . Each macroscopic point is identified through a position vector \bar{x}_i in $\bar{\mathcal{D}}$. On the other hand, the microscopic level (or unit cell) occupies the space \mathcal{D} , which is bounded by a surface $\partial \mathcal{D}$ with unit vector n_i . Each microscopic point in \mathcal{D} is identified through a position vector x_i . The two vectors \bar{x}_i and x_i are connected through the relation $x_i = \bar{x}_i/\epsilon$, where ϵ denotes the characteristic length of the microstructure. When considering the composite as a whole, the general coordinate system x_i^{ϵ} is utilized. Moreover, the following scale separation rule holds:

$$\frac{\partial}{\partial x_i^{\epsilon}} = \frac{\partial}{\partial \bar{x}_i} + \frac{1}{\epsilon} \frac{\partial}{\partial x_i}.$$
 (1)

All the variables that correspond to the general composite response are defined with a superscript ϵ . Additionally, a bar above a symbol denotes a macroscopic variable which depends only on the vector \bar{x}_i . Also, the operator $\langle \{\bullet\} \rangle$ stands for the volume average over the unit cell. Finally, a dot above a quantity defines the total derivative of the quantity with respect to time.

Table 1 illustrates the conservation laws and the kinematics of the studied problem. In this Table u_i^{ϵ} denotes the displacement vector, $\varepsilon_{ij}^{\epsilon}$ is the strain tensor, σ_{ij}^{ϵ} is the stress tensor, θ^{ϵ} is the absolute temperature and $\nabla \theta_i^{\epsilon}$ is the temperature gradient. Moreover q_i^{ϵ} , U^{ϵ} and s^{ϵ} denote the heat flux vector, the internal energy and the specific entropy per unit volume respectively. Body forces and internal forces, as well as sources of heat radiation are ignored.

To account for a specific type of material, one needs to express the internal energy in terms of certain variables that dictate the status of the material at each time instant. Apart from the strain and the entropy, a set of internal variables could be necessary to describe the material state. Thus, one can choose an internal energy of the general form

$$U^{\epsilon} := U^{\epsilon}(\varepsilon_{ij}^{\epsilon}, s^{\epsilon}, \zeta_{\alpha}^{\epsilon}), \tag{2}$$

Equation	expression
Kinematics	$\varepsilon_{ij}^{\epsilon} = \frac{1}{2} \left[\frac{\partial u_i^{\epsilon}}{\partial x_j^{\epsilon}} + \frac{\partial u_j^{\epsilon}}{\partial x_i^{\epsilon}} \right]$
Equilibrium	$\frac{\partial \sigma_{ij}^{\epsilon}}{\partial x_{j}^{\epsilon}} = 0$
energy balance	$\frac{\partial q_i^{\epsilon}}{\partial x_i^{\epsilon}} = \sigma_{ij}^{\epsilon} \dot{\varepsilon}_{ij}^{\epsilon} - \dot{U}^{\epsilon}$
entropy inequality	$\theta^{\epsilon}\dot{s}^{\epsilon} + \sigma_{ij}^{\epsilon}\dot{\varepsilon}_{ij}^{\epsilon} - \dot{U}^{\epsilon} - \frac{1}{\Omega\epsilon}q_{i}^{\epsilon}\nabla\theta_{i}^{\epsilon} \geq 0$

Table 1. Kinematics and conservation laws of the fully coupled thermomechanical problem.

where $\zeta_{\alpha}^{\epsilon}$ stands for the list of the scalars z^{ϵ} , vectors z_{i}^{ϵ} and second order tensors z_{ij}^{ϵ} internal variables of all the composite constituents. For simplicity, the following operator is introduced:

$$\frac{\partial \{\bullet\}}{\partial \zeta_{\alpha}} \dot{\zeta}_{\alpha} = \sum_{m} \frac{\partial \{\bullet\}}{\partial z^{(m)}} \dot{z}^{(m)} + \sum_{n} \frac{\partial \{\bullet\}}{\partial z_{i}^{(n)}} \dot{z}_{i}^{(n)} + \sum_{q} \frac{\partial \{\bullet\}}{\partial z_{ij}^{(q)}} \dot{z}_{ij}^{(q)}. \tag{3}$$

Identifying constitutive laws in terms of entropy is not practical, so it is more convenient to introduce alternative potentials. The Helmholtz free energy potential is written as

$$\Psi^{\epsilon} := \Psi^{\epsilon}(\varepsilon_{ii}^{\epsilon}, \theta^{\epsilon}, \zeta_{\alpha}^{\epsilon}), \quad \text{with} \quad \Psi^{\epsilon} = U^{\epsilon} - s^{\epsilon}\theta^{\epsilon}. \tag{4}$$

According to the classical approach and assumptions of thermodynamics, the following relations are obtained:

$$\sigma_{ij}^{\epsilon} = \frac{\partial \Psi^{\epsilon}}{\partial \varepsilon_{ij}^{\epsilon}}, \quad s^{\epsilon} = -\frac{\partial \Psi^{\epsilon}}{\partial \theta^{\epsilon}}, \quad \gamma_{\text{loc}}^{\epsilon} = \Xi_{\alpha}^{\epsilon} \, \dot{\zeta}_{\alpha}^{\epsilon}, \quad \Xi_{\alpha}^{\epsilon} = -\frac{\partial \Psi^{\epsilon}}{\partial \zeta_{\alpha}^{\epsilon}}, \tag{5}$$

where γ_{loc} denotes local dissipation due to mechanical work and Ξ_{α}^{ϵ} represent the thermodynamic forces. With the help of these relations the second law and the rate of the Helmholtz free energy potential take the forms

$$\gamma_{\text{loc}}^{\epsilon} - \frac{1}{\theta^{\epsilon}} q_{i}^{\epsilon} \nabla \theta_{i}^{\epsilon} \ge 0, \quad \dot{\Psi}^{\epsilon} = \sigma_{ij}^{\epsilon} \dot{\varepsilon}_{ij}^{\epsilon} - s^{\epsilon} \dot{\theta}^{\epsilon} - \Xi_{\alpha}^{\epsilon} \dot{\zeta}_{\alpha}^{\epsilon} = \sigma^{\epsilon} \dot{\varepsilon}_{ij}^{\epsilon} - s^{\epsilon} \dot{\theta}^{\epsilon} - \gamma_{\text{loc}}^{\epsilon}. \tag{6}$$

According to the AEH method, the periodicity of the composite microstructure allows to assume that all the implicated variables can be expressed with the help of an asymptotic series expansion:

$$u_{i}^{\epsilon}(x_{k}^{\epsilon}) = \bar{u}_{i}(\bar{x}_{k}, x_{k}) + \epsilon u_{i}^{(1)}(\bar{x}_{k}, x_{k}) + ..., \qquad \theta^{\epsilon}(x_{k}^{\epsilon}) = \bar{\theta}(\bar{x}_{k}, x_{k}) + \epsilon \theta^{(1)}(\bar{x}_{k}, x_{k}) + ..., \qquad \theta^{\epsilon}(x_{k}^{\epsilon}) = \bar{\theta}(\bar{x}_{k}, x_{k}) + \epsilon \theta^{(1)}(\bar{x}_{k}, x_{k}) + ..., \qquad \theta^{\epsilon}(x_{k}^{\epsilon}) = \bar{\theta}(\bar{x}_{k}, x_{k}) + \epsilon \theta^{(1)}(\bar{x}_{k}, x_{k}) + ..., \qquad \theta^{\epsilon}(x_{k}^{\epsilon}) = \bar{\theta}(\bar{x}_{k}, x_{k}) + \epsilon \theta^{(1)}(\bar{x}_{k}, x_{k}) + ..., \qquad \theta^{\epsilon}(x_{k}^{\epsilon}) = \bar{\theta}(\bar{x}_{k}, x_{k}) + \epsilon \theta^{(1)}(\bar{x}_{k}, x_{k}) + ..., \qquad \theta^{\epsilon}(x_{k}^{\epsilon}) = \bar{\theta}(\bar{x}_{k}, x_{k}) + \epsilon \theta^{(1)}(\bar{x}_{k}, x_{k}) + ..., \qquad \theta^{\epsilon}(x_{k}^{\epsilon}) = \bar{\theta}(\bar{x}_{k}, x_{k}) + \epsilon \theta^{(1)}(\bar{x}_{k}, x_{k}) + ..., \qquad \theta^{\epsilon}(x_{k}^{\epsilon}) = \bar{\theta}(\bar{x}_{k}, x_{k}) + \epsilon \theta^{(1)}(\bar{x}_{k}, x_{k}) + ..., \qquad \theta^{\epsilon}(x_{k}^{\epsilon}) = \bar{\theta}(\bar{x}_{k}, x_{k}) + \epsilon \theta^{(1)}(\bar{x}_{k}, x_{k}) + ..., \qquad \theta^{\epsilon}(x_{k}^{\epsilon}) = \bar{\theta}(\bar{x}_{k}, x_{k}) + \epsilon \theta^{(1)}(\bar{x}_{k}, x_{k}) + ..., \qquad \theta^{\epsilon}(x_{k}^{\epsilon}) = \bar{\theta}(\bar{x}_{k}, x_{k}) + \epsilon \theta^{(1)}(\bar{x}_{k}, x_{k}) + ..., \qquad \theta^{\epsilon}(x_{k}^{\epsilon}) = \bar{\theta}(\bar{x}_{k}, x_{k}) + \epsilon \theta^{(1)}(\bar{x}_{k}, x_{k}) + ..., \qquad \theta^{\epsilon}(x_{k}^{\epsilon}) = \bar{\theta}(\bar{x}_{k}, x_{k}) + \epsilon \theta^{(1)}(\bar{x}_{k}, x_{k}) + ..., \qquad \theta^{\epsilon}(x_{k}^{\epsilon}) = \bar{\theta}(\bar{x}_{k}, x_{k}) + \epsilon \theta^{(1)}(\bar{x}_{k}, x_{k}) + ..., \qquad \theta^{\epsilon}(x_{k}^{\epsilon}) = \bar{\theta}(\bar{x}_{k}, x_{k}) + \epsilon \theta^{(1)}(\bar{x}_{k}, x_{k}) + ..., \qquad \theta^{\epsilon}(x_{k}^{\epsilon}) = \bar{\theta}(\bar{x}_{k}, x_{k}) + \epsilon \theta^{(1)}(\bar{x}_{k}, x_{k}) + ..., \qquad \theta^{\epsilon}(x_{k}^{\epsilon}) = \bar{\theta}(\bar{x}_{k}, x_{k}) + \epsilon \theta^{(1)}(\bar{x}_{k}, x_{k}) + ..., \qquad \theta^{\epsilon}(x_{k}^{\epsilon}) = \bar{\theta}(\bar{x}_{k}, x_{k}) + \epsilon \theta^{(1)}(\bar{x}_{k}, x_{k}) + ..., \qquad \theta^{\epsilon}(x_{k}^{\epsilon}) = \bar{\theta}(\bar{x}_{k}, x_{k}) + \epsilon \theta^{(1)}(\bar{x}_{k}, x_{k}) + ..., \qquad \theta^{\epsilon}(x_{k}^{\epsilon}) = \bar{\theta}(\bar{x}_{k}, x_{k}) + \epsilon \theta^{(1)}(\bar{x}_{k}, x_{k}) + ..., \qquad \theta^{\epsilon}(x_{k}^{\epsilon}) = \bar{\theta}(\bar{x}_{k}, x_{k}) + \epsilon \theta^{(1)}(\bar{x}_{k}, x_{k}) + ..., \qquad \theta^{\epsilon}(x_{k}^{\epsilon}) = \bar{\theta}(\bar{x}_{k}, x_{k}) + \epsilon \theta^{(1)}(\bar{x}_{k}, x_{k}) + ..., \qquad \theta^{\epsilon}(\bar{x}_{k}, x_{k}) + \bar{\theta}(\bar{x}_{k}, x_{k}) + \bar{\theta}(\bar{x}_{k}, x_{k}) + \bar{\theta}(\bar{x}_{k}, x_{k}) + ..., \qquad \theta^{\epsilon}(\bar{x}_{k}, x_{k}) + \bar{\theta}(\bar{x}_{k}, x_{k}) + \bar{\theta}(\bar{x}_{k}, x_{k}) + \bar{\theta}(\bar{x}_{k}, x_{k}) + \bar{\theta}(\bar{x}_{k},$$

where all two-scale functions $\{\bullet\}^{(0)}$, $\{\bullet\}^{(1)}$ e.t.c. are periodic in x_i . After applying this substitutions to all the problem equations, and with proper mathematical treatment, one finally obtains the results presented in Tables 2 and 3 [6].

As it can be observed from the obtained results, the internal variables and their conjugate thermodynamic forces are well defined in the unit cell. This unfortunately is not true for the macroscale problem. The averaged term $\left\langle\Xi_{\alpha}^{(0)}\ \dot{\zeta}_{\alpha}^{(0)}\right\rangle$ cannot be decomposed into a macroscopic variables product, like the rest of the terms. Only the average of $\gamma_{\rm loc}^{(0)}$ can be identified as the macroscopic $\bar{\gamma}_{\rm loc}$. Thus, the mechanical dissipation in the macroscale can be obtained only by averaging the microscale mechanical dissipation over the unit cell, causing problems in expressing analytically the macroscopic energy equation. One way to overcome this difficulty is to consider a linearized, incremental form of the fully coupled thermomechanical problem.

variable	microscale	macroscale
strain	$arepsilon_{ij}^{(0)}$	$\bar{\varepsilon}_{ij} = \left\langle \varepsilon_{ij}^{(0)} \right\rangle$
stress	$\sigma^{(0)}_{ij}$	$\overline{\sigma}_{ij} = \left\langle \sigma_{ij}^{(0)} \right\rangle$
temperature gradient	$ abla heta_i^{(0)}$	$\overline{\nabla \theta}_i = \left\langle \nabla \theta_i^{(0)} \right\rangle$
heat flux	$q_i^{(0)}$	$\bar{q}_i = \left\langle q_i^{(0)} \right\rangle$
specific entropy per unit volume	$s^{(0)}$	$\bar{s} = \left\langle s^{(0)} \right\rangle$
internal energy per unit volume	$U^{(0)}$	$\overline{U} = \left\langle U^{(0)} \right\rangle$
Helmholtz free energy potential	$\Psi^{(0)}\left(arepsilon_{ij}^{(0)},ar{ heta},\zeta_{lpha}^{(0)} ight)$	$\overline{\Psi} = \left\langle \Psi^{(0)} \right\rangle$
intrinsic dissipation	$\gamma_{\rm loc}^{(0)}=\Xi_\alpha^{(0)}\ \dot\zeta_\alpha^{(0)}$	$\bar{\gamma}_{\mathrm{loc}} = \left\langle \gamma_{\mathrm{loc}}^{(0)} \right\rangle$

Table 3. Microscale and macroscale equations

equation	microscale	macroscale
kinematics	$\varepsilon_{ij}^{(0)} = \bar{\varepsilon}_{ij} + \frac{1}{2} \left[\frac{\partial u_i^{(1)}}{\partial x_j} + \frac{\partial u_j^{(1)}}{\partial x_i} \right]$	$\bar{\varepsilon}_{ij} = \frac{1}{2} \left[\frac{\partial \bar{u}_i}{\partial \bar{x}_j} + \frac{\partial \bar{u}_j}{\partial \bar{x}_i} \right]$
equilibrium	$\frac{\partial \sigma_{ij}^{(0)}}{\partial x_j} = 0$	$\frac{\partial \overline{\sigma}_{ij}}{\partial \overline{x}_j} = 0$
temperature gradient	$\nabla \theta_i^{(0)} = \overline{\nabla \theta}_i + \frac{\partial \theta^{(1)}}{\partial x_i}$	$\overline{\nabla}\overline{\theta}_i = \frac{\partial\overline{\theta}}{\partial\overline{x}_i}$
energy equation	$\frac{\partial q_i^{(0)}}{\partial x_i} = 0$	$\frac{\partial \bar{q}_i}{\partial \bar{x}_i} = \bar{\sigma}_{ij} \dot{\bar{\varepsilon}}_{ij} - \dot{\bar{U}}$
entropy inequality	$\gamma_{\text{loc}}^{(0)} - \frac{1}{\bar{\theta}} q_i^{(0)} \nabla \theta_i^{(0)} \ge 0$	$\bar{\gamma}_{\text{loc}} - \frac{1}{\bar{\theta}} \bar{q}_i \overline{\nabla \theta}_i \ge 0$
Helmholtz-internal energy	$\Psi^{(0)} = U^{(0)} - s^{(0)}\bar{\theta}$	$\overline{\Psi} = \overline{U} - \overline{s}\overline{\theta}$

3. Linearized, incremental formulation

In many dissipative materials the relation between the stress, the strain, the temperature and the internal variables is very complicated and is provided only in implicit form. In computational, incremental formulations for nonlinear constitutive laws, one needs to linearize initially the real problem in time and then to proceed to a second linearization of the nonlinear expressions. An effective approach that utilizes this technique is the well known return mapping algorithm (RMA) scheme [7]. For homogeniza-

tion problems under small deformations, extension of the RMA has been proposed in the literature for elastoplastic [8] and shape memory alloy composites [9]. In brief, the macroscale and the microscale (unit cell) problems are solved simultaneously, using an iterative scheme: from the macroscale analysis the macroscopic strains, temperatures and tamperature gradients are calculated, which in turn are used in the unit cell problem to compute the microscale variables and the rest of the unknown macroscopic variables (stresses, heat fluxes e.t.c.). Moreover, the unit cell problem is utilized to compute the macroscopic tangent moduli, which are required for the macroscale problem.

In the RMA framework there are two types of increments of a quantity x: a) increment in time, denoted by Δx and b) increment during the Newton-Raphson scheme in the linearized equations, denoted by the δx . Following this notation, the main equations of the unit cell problem (kinematics and conservation laws) are written in the linearized, incremental form as

$$\delta \varepsilon_{ij}^{(0)} = \delta \overline{\varepsilon}_{ij} + \frac{1}{2} \left[\frac{\partial \delta u_i^{(1)}}{\partial x_j} + \frac{\partial \delta u_j^{(1)}}{\partial x_i} \right], \quad \delta \nabla \theta_i^{(0)} = \delta \overline{\nabla} \theta_i + \frac{\partial \delta \theta^{(1)}}{\partial x_i},$$

$$\frac{\partial}{\partial x_i} (\sigma_{ij}^{(0)} + \delta \sigma_{ij}^{(0)}) = 0, \quad \frac{\partial}{\partial x_i} \left(q_i^{(0)} + \delta q_i^{(0)} \right) = 0.$$
(8)

These equations are accompanied by the constitutive law, which provides the increments of the stress tensor $\sigma_{ij}^{(0)}$ and the quantity $r^{(0)} = \sigma_{ij}^{(0)} \dot{\varepsilon}_{ij}^{(0)} - \dot{U}^{(0)}$. Both of these quantities depend on the microscopic Helmholtz energy potential, which is a function of the strain $\varepsilon_{ij}^{(0)}$, the temperature $\bar{\theta}$ and the internal variables. In RMA, after proper algebraic treatment of the linearized expressions, the increments of the internal variables can be expressed in terms of the increments of strain and temperature. Thus, the linearized constitutive expressions can obtain the general forms

$$\delta\sigma_{ij}^{(0)} = D_{ijkl}^{\varepsilon} \delta\varepsilon_{kl}^{(0)} + D_{ij}^{\theta} \delta\bar{\theta}, \quad \delta r^{(0)} = R_{ij}^{\varepsilon} \delta\varepsilon_{ij}^{(0)} + R^{\theta} \delta\bar{\theta}, \quad \delta q_i^{(0)} = -\kappa_{ij} \delta\nabla\theta_j^{(0)}, \tag{9}$$

where D_{ijkl}^{ε} , D_{ij}^{θ} , R_{ij}^{ε} , R^{θ} denote the coupled thermomechanical tangent moduli and are assumed constant during the iteration step. Moreover κ_{ij} is the thermal conductivity tensor.

From the linearized system one obtains a) the macroscopic fields and b) appropriate macroscopic quantities of D_{ijkl}^{ε} , D_{ij}^{θ} , R_{ij}^{ε} , R^{θ} and κ_{ij} , which are essential for the solution of the macroscopic problem. To achieve this, a two-step approach is followed:

1. At the first step, the macrostrain tensor, the macrotemperature and the macrotemperature gradient are provided exclusively by the macroscale problem, and the terms $\delta \bar{\varepsilon}_{ij}$, $\delta \bar{\theta}$ and $\delta \overline{\nabla} \bar{\theta}_i$ are set to zero. Then $(8)_{3,4}$ are reduced to

$$\frac{\partial}{\partial x_j} \left(\sigma_{ij}^{(0)} + D_{ijkl}^{\varepsilon} \frac{\partial \delta u_k^{(1)}}{\partial x_l} \right) = 0, \qquad \frac{\partial}{\partial x_i} \left(q_i^{(0)} - \kappa_{ij} \frac{\partial \delta \theta^{(1)}}{\partial x_j} \right) = 0, \tag{10}$$

which can be solved iteratively. When the numerical convergence is achieved, the time increments and the actual values of the fluctuating terms $u_i^{(1)}$ and $\theta^{(1)}$ are obtained. Thus, all the microscopic quantities and their averaged (macroscopic) counterparts are computed.

2. When the first step is completed, the residual terms are assumed exactly zero and the terms $\delta \bar{\varepsilon}_{ij}$, $\delta \bar{\theta}$ and $\delta \nabla \bar{\theta}_i$ are 'released' from being zero. Using this assumption the microscale equations are written as

$$\frac{\partial}{\partial x_{j}} \left(D_{ijkl}^{\varepsilon} \delta \bar{\varepsilon}_{kl} + D_{ij}^{\theta} \delta \bar{\theta} + D_{ijkl}^{\varepsilon} \frac{\partial \delta u_{k}^{(1)}}{\partial x_{l}} \right) = 0, \quad \frac{\partial}{\partial x_{i}} \left(\kappa_{ij} \delta \overline{\nabla \theta}_{j} + \kappa_{ij} \frac{\partial \delta \theta^{(1)}}{\partial x_{j}} \right) = 0, \quad (11)$$

where the microscopic tensors D^{ε}_{ijkl} and D^{θ}_{ij} are the last values obtained from the previous step. The solution of the above homogeneous system is written in the form

$$\delta u_i^{(1)} = \delta \bar{\varepsilon}_{kl} \chi_{kli}^{\varepsilon} + \delta \bar{\theta} \chi_i^{\theta}, \quad \delta \theta^{(1)} = \delta \overline{\nabla} \theta_i \psi_i^{\theta}, \tag{12}$$

where the third order tensor χ_{kli}^{ε} and the vectors χ_{i}^{θ} , ψ_{i}^{θ} are called corrector terms and they are calculated from the auxiliary linear equations

$$\frac{\partial}{\partial x_j} \left(D_{ijkl}^{\varepsilon} + D_{ijmn}^{\varepsilon} \frac{\partial \chi_{klm}^{\varepsilon}}{\partial x_n} \right) = 0, \quad \frac{\partial}{\partial x_j} \left(D_{ij}^{\theta} + D_{ijkl}^{\varepsilon} \frac{\partial \chi_k^{\theta}}{\partial x_l} \right) = 0, \quad \frac{\partial}{\partial x_i} \left(\kappa_{ij} + \kappa_{ik} \frac{\partial \psi_j^{\theta}}{\partial x_k} \right) = 0. \tag{13}$$

Using the solution (12), the increments of the various microscopic fields are written as

$$\delta\varepsilon_{ij}^{(0)} = A_{ijkl}^{\varepsilon}\delta\bar{\varepsilon}_{kl} + A_{ij}^{\theta}\delta\bar{\theta}, \quad \delta\nabla\theta_{i}^{(0)} = \Theta_{ij}\delta\overline{\nabla}\theta_{j},$$

$$\delta\sigma_{ij}^{(0)} = D_{ijmn}^{\varepsilon}A_{mnkl}^{\varepsilon}\delta\bar{\varepsilon}_{kl} + \left[D_{ij}^{\theta} + D_{ijkl}^{\varepsilon}A_{kl}^{\theta}\right]\delta\bar{\theta}, \quad \delta q_{i}^{(0)} = -\kappa_{ik}\Theta_{kj}\delta\overline{\nabla}\theta_{j},$$

$$\delta r^{(0)} = R_{kl}^{\varepsilon}A_{klij}^{\varepsilon}\delta\bar{\varepsilon}_{ij} + \left[R^{\theta} + R_{ij}^{\varepsilon}A_{ij}^{\theta}\right]\delta\bar{\theta},$$

$$A_{ijkl}^{\varepsilon} = I_{ijkl} + \frac{1}{2}\left[\frac{\partial\chi_{kli}^{\varepsilon}}{\partial x_{j}} + \frac{\partial\chi_{klj}^{\varepsilon}}{\partial x_{i}}\right], \quad A_{ij}^{\theta} = \frac{1}{2}\left[\frac{\partial\chi_{i}^{\theta}}{\partial x_{j}} + \frac{\partial\chi_{j}^{\theta}}{\partial x_{i}}\right], \quad \Theta_{ij} = I_{ij} + \frac{\partial\psi_{j}^{\theta}}{\partial x_{i}}.$$

$$(14)$$

In the above expressions I_{ijkl} denotes the fourth order symmetric identity tensor and I_{ij} is the second order identity tensor. Averaging these fields over the unit cell gives the macroscopic tensors

$$\overline{D}_{ijkl}^{\varepsilon} = \left\langle D_{ijmn}^{\varepsilon} A_{mnkl}^{\varepsilon} \right\rangle, \quad \overline{D}_{ij}^{\theta} = \left\langle D_{ij}^{\theta} + D_{ijkl}^{\varepsilon} A_{kl}^{\theta} \right\rangle, \quad \overline{\kappa}_{ij} = \left\langle \kappa_{ik} \Theta_{kj} \right\rangle,
\overline{R}_{ij}^{\varepsilon} = \left\langle R_{kl}^{\varepsilon} A_{klij}^{\varepsilon} \right\rangle, \quad \overline{R}^{\theta} = \left\langle R^{\theta} + R_{ij}^{\varepsilon} A_{ij}^{\theta} \right\rangle.$$
(15)

The information obtained from these two steps are sufficient to pass to the macroscale analysis and compute the next values of $\delta \bar{\varepsilon}_{ij}$, $\delta \bar{\theta}$ and $\delta \bar{\nabla} \theta_i$.

4. Numerical example

The example presented here illustrates the response of a viscoplastic multilayered composite under coupled thermomechanical loading conditions. An epoxy, with volume fraction 20%, and a metal, with volume fraction 80% are bonded, forming a multilayered structure which is repeated periodically in the overall composite. The epoxy behaves elastically, while the steel 316 is considered as a viscoplastic material.

The advantage of the multilayered composite is that the unit cell problem has a semi-analytical solution. Thus, the global thermomechanical response of the composite structure can be directly computed through a finite element analysis (FE), using as "material law" the semi-analytical solution for multilayered composites. This solution is introduced in a specially designed User Material subroutine (UMAT) for the commercial finite element software ABAOUS.

Numerical calculations are performed on the macroscale, which is defined by a cubic specimen with dimensions 1 cm \times 1 cm \times 1 cm. 1000 C3D8T elements (8 node, 3-D solid elements for coupled temperature-displacement analysis) are utilized to represent the macrostructure. Fig. 1 demonstrates the problem in both macro- and microscale. The loading conditions are the following: Initially, the

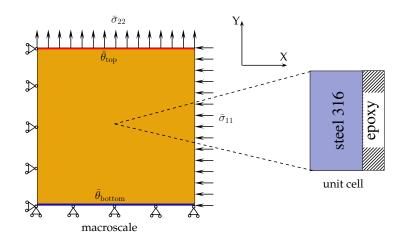


Figure 1. Write your figure caption here.

temperature of the structure is set to 293.15°K. The displacement is fixed in the Y direction of the bottom surface, the Z direction of the front surface and the X direction of the left surface. The temperature $\bar{\theta}_{bottom}$ of the bottom surface remains constant with time, equal to 293.15°K. The duration of the test is 200 s. During this time the specimen is undergoing i) a linearly increasing tensile stress $\bar{\sigma}_{22}$ with time, up to 150 MPa, on the upper surface, ii) a linearly increasing compressive stress $\bar{\sigma}_{11}$ with time, up to 150 MPa, on the right surface, and iii) a linearly increasing temperature $\bar{\theta}_{top}$ with time, up to 303.15°K, on the top surface. Fig. 2 illustrates the temperature profile of the specimen and the mechanical response, at a macroscopic point, of the epoxy, the metal and the overall composite at the end of the calculations.

5. Conclusion

The theoretical and numerical framework developed in this work is capable of identifying the fully coupled thermomechanical response of periodic composites with arbitrary nonlinear material phases. The new framework can be used for studying composites where the interaction between mechanical and thermal fields is strong and fully coupled thermomechanical analysis is unavoidable (for instance, in polymeric composites with viscoelastic or viscoplastic behavior, whose mechanical properties are very sensitive to temperature changes).

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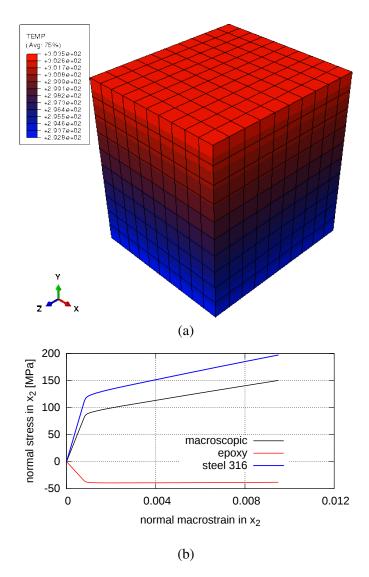


Figure 2. (a) Temperature distribution in the specimen and (b) mechanical behavior, at a macroscopic point, of the material constituents and the overall composite.

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