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Overall thermomechanical properties of layered materials for energy devices applications

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ABSTRACT

This paper is concerned with the analysis of effective thermomechanical properties of multi-layered materials of interest for solid oxide fuel cells (SOFC) and lithium ions batteries fabrication. The recently developed asymptotic homogenization procedure is applied in order to express the overall thermoelastic constants of the first order equivalent continuum in terms of microfluctuations functions, and these functions are obtained by the solution of the corresponding recursive *cell problems*. The effects of thermal stresses on periodic multi-layered thermoelastic composite reproducing the characteristics of solid oxide fuel cells (SOFC-like) are studied assuming periodic body forces and heat sources, and the solution derived by means of the asymptotic homogenization approach is compared with the results obtained by finite elements analysis of the associate heterogeneous material.

1. Introduction

Solid oxide fuel cells (SOFC) and lithium ions batteries are two of the most performing and promising battery devices which can play an important role in realizing efficient small-scale power generation systems providing renewable energy for industrial applications. Due to the high temperatures which can be reached in operative scenarios [37], the components of such batteries are subject to severe thermomechanical stresses which can cause damage and crack formation, compromising the performance of the devices in terms of power generation and energy conversion efficiency [4,23]. Modelling the thermomechanical properties of SOFCs devices and lithium ions batteries represent a crucial issue in order to predict these phenomena and then to ensure the successful manufacture and the reliability of the systems.

Both SOFCs and lithium ions batteries are characterized by a multi-layered configuration possessing many phases of composite materials, where the elementary cell is represented by the anode-electrolyte-cathode system. Moreover, in many operative situations solid oxide fuel cells are organized in stacks where several anode-electrolyte-cathode systems are separated by metallic interconnections. Since the macroscopic behaviour of these multi-layered structures is influenced by phenomena occurring at scale-lengths characteristic of the microscopic constituents, which is small compared to the macroscopic dimension (i.e. structural size), multiscale modelling of SOFCs and lithium ions batteries implies challenging numerical computations which require very fine mesh of finite elements and then strong computational resources [38,30]. Homogenization techniques represent an useful and advantageous method for providing a rigorous and synthetic description of the effects of the microscopic phases on the overall properties of the materials. The application of these approaches makes possible to avoid the challenging numerical computations required by computational modelling of heterogeneous media, and are particularly suitable for periodic composite media, such as multi-layered battery devices. Several homogenization techniques have been proposed for studying overall properties of composite materials, such as the asymptotic (see for example [39–41,18,17,29,2,20,34,19,3,44]), the variational-asymptotic methods (see for example [43,36,42,8,14]) and the computational approaches (see for example [27,26,32,33,31,28,9,10,22,1,5–7]).

The principal aim of this article is to provide exact closed-form expressions to estimate the overall thermoelastic and heat conduction tensors of multi-layered battery devices avoiding the challenging computations required by standard numerical modelling of the heterogeneous structures [21]. With this purpose, an ideal periodic multi-layered thermoelastic composite material reproducing the planar geometry of an idealized battery device is introduced (see Fig. 1). The thermoelastic and heat conduction tensors of the first order continuum equivalent to the introduced multi-layered battery-like thermoelastic composite are derived applying the asymptotic homogenization approach recently developed by [16] for studying heterogeneous media in presence of

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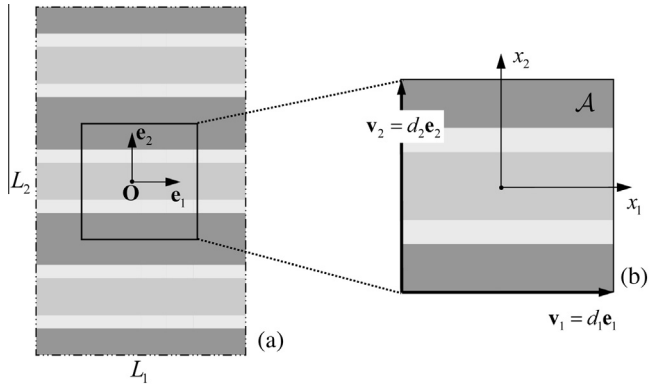

Fig. 1. (a) Heterogeneous material – Periodic domain L; (b) Periodic cell $\mathcal{A}$ and periodicity vectors.

thermodiffusive phenomena. Following the rigorous procedure developed in [17,43,12–14,11,8] for composite elastic media with periodic microstructures and generalized by [16] to the case of thermodiffusive materials, the fields equation for the homogenized first order thermoelastic continuum equivalent to the multi-layered battery devices are derived, and exact expressions for the overall thermoelastic constants of this equivalent medium are obtained. These expressions are used to determine analytically the components of the overall elastic, thermoelastic and heat conduction tensors corresponding to a tri-phase layered thermoelastic composite of interests for SOFCs devices fabrication. The thermoelastic constants of the three phases are assumed to possess values typical of the constituents of real SOFCs devices, evaluated by means of accurate experimental techniques and homogenization methods and accounting for the microstructure, such as the porosity, of the electrolyte and the electrodes. The fields equation of the first order equivalent thermoelastic media are solved considering periodic heat sources, which localized and unlocalized profiles are representative for modelling some thermal effects detected in real situations. The solution of the homogenized field equations is compared with the numerical results obtained by the heterogeneous model assuming periodic body force and heat and mass sources acting on the considered three-phase layered composite.

The article is organized as follows: in Section 2 the geometry of the idealized periodic thermoelastic battery-like material is illustrated, and the corresponding constitutive relations and balance equations are introduced. The developed multi-scale asymptotic homogenization technique is described in Section 3, based on down-scaling relations correlating the microscopic fields to the macroscopic displacements and temperature. The unknown perturbation functions describing the effects of the material heterogeneities are defined as solutions of the corresponding non-homogeneous cell problems. In the same Section, the fields equations and explicit expressions for the components of the elastic, thermoelastic and heat conduction tensors of the equivalent first order homogeneous continuum are derived. In Section 4, these results are used for studying overall properties of three-phase layered thermoelastic composites of interests for SOFCs devices fabrication, represented by an idealized cathode-electrolyte-anod e-interconnection system. Finally, a critical discussion about the obtained results is reported together with conclusions and future perspectives in Section 5.

2. Multiscale modelling of periodic thermoelastic composites

Many energy battery devices such as lithium ions batteries and solid oxide fuel cells (SOFC) are characterized by multi-layered structures [35,24,25]. In order to develop a general approach for estimating effective thermomechanical properties of both lithium ions batteries and solid oxide fuel cells, we introduce a periodic multi-layered thermoelastic composite media reproducing the planar geometry of an idealized battery device as shown in Fig. 1.

The constituent elements of the medium are modelled as a linear thermoelastic Cauchy continuum subject to small strains. The material point is identified by position vector $\boldsymbol{x} = x_1\boldsymbol{e}_1 + x_2\boldsymbol{e}_2$ referred to a system of coordinates with origin at point O and orthogonal base $\{\boldsymbol{e}_1, \boldsymbol{e}_2\}$. Fig. 1b shows the periodic cell $\mathcal{A} = [0, \varepsilon] \times [0, \delta\varepsilon]$ with characteristic size ε. The entire periodic medium can be obtained spanning the cell $\mathcal{A}$ by the two orthogonal vectors $\boldsymbol{v}_1 = d_1\boldsymbol{e}_1 = \varepsilon\boldsymbol{e}_1, \boldsymbol{v}_2 = d_2\boldsymbol{e}_2 = \delta\varepsilon\boldsymbol{e}_2$. $\mathcal{A}$ represents the elementary cell period of the elasticity tensor $\mathbb{C}^{(m,\varepsilon)}(\boldsymbol{x})$, the heat conduction tensor $\boldsymbol{K}^{(m,\varepsilon)}(\boldsymbol{x})$ and the thermal dilatation tensor $\boldsymbol{\alpha}^{(m,\varepsilon)}(\boldsymbol{x})$, which are defined as follows

$$\mathbb{C}^{(m,\varepsilon)}(\boldsymbol{x} + \boldsymbol{v}_i) = \mathbb{C}^{(m,\varepsilon)}(\boldsymbol{x}), \quad i = 1,2, \ \forall \boldsymbol{x} \in \mathcal{A}. \tag{1}$$

$$\boldsymbol{K}^{(m,\varepsilon)}(\boldsymbol{x} + \boldsymbol{v}_i) = \boldsymbol{K}^{(m,\varepsilon)}(\boldsymbol{x}), \quad \boldsymbol{\alpha}^{(m,\varepsilon)}(\boldsymbol{x} + \boldsymbol{v}_i) = \boldsymbol{\alpha}^{(m,\varepsilon)}(\boldsymbol{x}), \quad i = 1,2, \ \forall \boldsymbol{x} \in \mathcal{A}. \tag{2}$$

The tensors (1) and (2) are commonly referred to as $\mathcal{A}$-periodic functions.

The system is subject to body forces $\boldsymbol{b}(\boldsymbol{x})$ and heat sources $r(\boldsymbol{x})$ which are assumed to be $\mathcal{L}$-periodic with period $\mathcal{L} = [0, L] \times [0, \delta L]$ and to have vanishing mean values on $\mathcal{L}$. Since L is a large multiple of ε, then $\mathcal{L}$ can be assumed to be a representative portion of the overall body. This means that $\boldsymbol{b}(\boldsymbol{x})$ and $r(\boldsymbol{x})$ possess a period much greater than the microstructural size ε.

A non-dimensional unit cell $\mathcal{Q} = [0, 1] \times [0, \delta]$ that reproduces the periodic microstructure by rescaling with the small parameter ε is introduced [8]. Two distinct scales are represented by the macroscopic (slow) variables $\boldsymbol{x} \in \mathcal{A}$ and the microscopic (fast) variable $\boldsymbol{\xi} = \boldsymbol{x}/\varepsilon \in \mathcal{Q}$ (see for example [17,43]). The constitutive tensors (1) and (2) are functions of the microscopic variable, whereas the body forces and heat sources depend on the slow macroscopic variable. Consequently, the mapping of both the elasticity and thermodiffusive tensors may be defined on $\mathcal{Q}$ as follows: $\mathbb{C}^{(m,\varepsilon)}(\boldsymbol{x}) = \mathbb{C}^m(\boldsymbol{\xi} = \boldsymbol{x}/\varepsilon)$, $\boldsymbol{K}^{(m,\varepsilon)}(\boldsymbol{x}) = \boldsymbol{K}^m(\boldsymbol{\xi} = \boldsymbol{x}/\varepsilon)$, $\boldsymbol{\alpha}^{(m,\varepsilon)}(\boldsymbol{x}) = \boldsymbol{\alpha}^m(\boldsymbol{\xi} = \boldsymbol{x}/\varepsilon)$, respectively.

The relevant microscopic fields are the micro-displacement $\boldsymbol{u}(\boldsymbol{x})$, and the microscopic temperature $\theta(\boldsymbol{x}) = T(\boldsymbol{x}) - T_0$ evaluated with respect to the natural state ($T = T_0$). The micro-stress $\boldsymbol{\sigma}(\boldsymbol{x})$ and the microscopic heat flux $\boldsymbol{q}(\boldsymbol{x})$ are defined by the following constitutive relations:

$$\boldsymbol{\sigma}(\boldsymbol{x}) = \mathbb{C}^m\left(\frac{\boldsymbol{x}}{\varepsilon}\right)\boldsymbol{\varepsilon}(\boldsymbol{x}) - \boldsymbol{\alpha}^m\left(\frac{\boldsymbol{x}}{\varepsilon}\right)\theta(\boldsymbol{x}), \tag{3}$$

$$\boldsymbol{q}(\boldsymbol{x}) = -\boldsymbol{K}^m\left(\frac{\boldsymbol{x}}{\varepsilon}\right)\nabla\theta(\boldsymbol{x}), \tag{4}$$

where $\boldsymbol{\varepsilon}(\boldsymbol{x}) = \mathrm{sym}\nabla\boldsymbol{u}(\boldsymbol{x})$ is the micro-strain tensor which is assumed to be zero at the fundamental state of the system. The micro-stresses (3) and the microscopic heat flux (4) satisfy the local balance equations on the domain $\mathcal{A}$

$$\nabla \cdot \boldsymbol{\sigma}(\boldsymbol{x}) + \boldsymbol{b}(\boldsymbol{x}) = \boldsymbol{0}, \tag{5}$$

$$\nabla \cdot \boldsymbol{q}(\boldsymbol{x}) - r(\boldsymbol{x}) = 0, \tag{6}$$

Substituting expressions (3) and (4) in Eqs. (5) and (6), and remembering the symmetry of the elasticity tensor, the resulting set of partial differential equations is written in the form

$$\nabla \cdot \left(\mathbb{C}^m\left(\frac{\boldsymbol{x}}{\varepsilon}\right)\nabla\boldsymbol{u}(\boldsymbol{x})\right) - \nabla \cdot \left(\boldsymbol{\alpha}^m\left(\frac{\boldsymbol{x}}{\varepsilon}\right)\theta(\boldsymbol{x})\right) + \boldsymbol{b}(\boldsymbol{x}) = \boldsymbol{0} \tag{7}$$