

Multiscale asymptotic homogenization analysis of thermo-diffusive composite materials

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December 31, 2015

Abstract

In this paper an asymptotic homogenization method for the analysis of composite materials with periodic microstructure in presence of thermodiffusion is described. Appropriate down-scaling relations correlating the microscopic fields to the macroscopic displacements, temperature and chemical potential are introduced. The effects of the material inhomogeneities are described by perturbation functions derived from the solution of recursive cell problems. Exact expressions for the overall elastic and thermodiffusive constants of the equivalent first order thermodiffusive continuum are derived. The proposed approach is applied to the case of a two-dimensional bi-phase orthotropic layered material, where the effective elastic and thermodiffusive properties can be determined analytically. Considering this illustrative example and assuming periodic body forces, heat and mass sources acting on the medium, the solution performed by the first order homogenization approach is compared with the numerical results obtained by the heterogeneous model.

Keywords: Periodic microstructure, Asymptotic homogenization, Thermodiffusion, Overall material properties.

1 Introduction

Composite materials are extensively used in industrial practice. Indeed, many advanced engineering applications, such as aerospace, aircraft, green building, biomedical, energetics and electronics require the design and the use of heterogeneous multiphase materials. Due to the microstructural effects as well as the interaction between their constituents, these materials may present several favorable physical properties, as for example high stiffness, improved strength and toughness, enhanced thermal conductivity, mass diffusivity or electrical permittivity.

Recently, multiphase composite materials have been largely used in the design and fabrication of battery devices, in particular of lithium-ion batteries and solid oxide fuel cells (Nakajo et al., 2012; Dev et al., 2014; Ellis et al., 2012). Since high operational temperatures can be reached and

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intense particle fluxes are needed for maintaining the electrical current, the components of such battery devices are subject to severe thermomechanical stresses as well as stresses induced by the particle diffusion, which can cause damage and crack formation, compromising the performance of the devices in terms of power generation and energy conversion efficiency (Atkinson and Sun, 2007; Delette et al., 2013). Modelling the mechanical and thermodiffusive properties of the components of such battery devices represent a crucial issue in order to predict these phenomena and then to ensure the successful manufacture and the reliability of the systems.

The macroscopic behavior of thermodiffusive composite materials used for realizing lithium-ion batteries and solid oxide fuel cells is influenced by multiphysics phenomena occurring at scale-lengths characteristic of the microscopic constituents, which is small compared to the macroscopic dimension (i.e. structural size) (Richardson et al., 2012; Bove and Ubertini, 2008; Hajimolana et al., 2011). Consequently, multiscale techniques represent an appropriate and powerful tool for modelling the effects of the microstructures on the macroscopic mechanical and thermodiffusive properties of these materials. In particular, for composites with periodic microstructures, 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.

Several homogenization techniques have been proposed for studying overall static and dynamic elastic properties of composite materials with periodic microstructures, such as the asymptotic (see for example Bensoussan et al. (1978); Bakhvalov and Panasenko (1984); Gambin and Kroner (1989); Allaire (1992); Boutin and Auriault (1993); Meguid and Kalamkarov (1994); Boutin (1996); Andrianov et al. (2008); Tran et al. (2012)), the variational-asymptotic methods (see for example Smyshlyaev and Cherednichenko (2000); Peerlings and Fleck (2004); Smyshlyaev (2009); Bacigalupo (2014); Bacigalupo and Gambarotta (2014)) and the computational approaches (see for example Forest and Sab (1998); Forest (2002); Kouznetsova et al. (2002, 2004); Kaczmarczyk et al. (2008); Forest and Trinh (2011); Bacigalupo and Gambarotta (2010, 2011, 2013); De Bellis and Addessi (2011); Addessi et al. (2013); Bacca et al. (2013a,b,c)). These techniques associate to the considered heterogeneous material at the micro-scale, described by a standard Cauchy continuum, an equivalent homogenous medium at the macro-scale. The behavior of the equivalent macroscopic material can be described by means of a first order continuum or alternatively a non-local medium. Multiscale asymptotic and computational homogenization procedures have been also proposed for the analysis of heterogeneous media in presence of multiphysics phenomena, such as thermomechanical (Kanouté et al., 2009; Zhang et al., 2007; Aboudi et al., 2001) and thermo-magneto-electro-elastic (Sixto-Camacho et al., 2013) deformations. Recently, these methods have been applied for studying the influence of the microstructural effects on the macroscopical mechanical behavior and operative performances of lithium-ion batteries (Salvadori et al., 2014) and solid oxide fuel cells (Bacigalupo et al., 2014). The overall properties of periodic multilayered structures characterizing such energy devices can be efficiently described by means of homogenization methods developed for periodic composite materials. Nevertheless, to the author's knowledge, a rigorous asymptotic procedure accounting for the effects of the microstructures on both macroscopic elastic and thermodiffusive properties of composite materials as well as on the coupling between these properties is still unknown in literature.

In this paper, an original asymptotic homogenization method for modelling the static elastic, thermal and diffusive properties of periodic thermodiffusive composite materials is proposed. The rigorous approach developed in Bakhvalov and Panasenko (1984); Smyshlyaev and Cherednichenko

(2000); Bacigalupo (2014) and Bacigalupo and Gambarotta (2014) is extended in order to account for the effects of the microstructures on the macroscopic temperature and chemical potential of the materials and on the stresses induced by these fields. The displacements, temperature and chemical potential at the micro- and macro-scale are related through an asymptotic expansion of the microscopic fields in terms of characteristic size ε of the microstructure. This expansion depends both on the macroscopic strains, temperature and chemical potential gradients and on unknown perturbation functions accounting for the effects of the heterogeneities. Perturbation functions representing the effects of the material microstructures on the displacement, temperature, chemical potential and on the coupling effects between these fields are introduced. These perturbation functions, depending only on the properties of the microstructure, are obtained through the solution of non-homogeneous problems on the cell with periodic boundary conditions.

Similarly to the procedure proposed in Smyshlyaev and Cherednichenko (2000) and Bacigalupo (2014), averaged field equations of infinite order are obtained, and their formal solution is performed by representing the macroscopic displacements, temperature and chemical potential in terms of power series. Field equation for the homogenized first order thermodiffusive continuum are derived, and exact expressions for the overall elastic and thermodiffusive constants of this equivalent medium are obtained. The proposed formulation is applied to the case of a two-dimensional bi-phase orthotropic layered material. The effective elastic and thermodiffusive constants corresponding to this example are determined analytically using the general expressions derived by the homogenization procedure. The solution performed by the proposed approach is compared with the numerical results obtained by the heterogeneous model assuming periodic body forces, heat and mass sources acting on the considered bi-phase layered composite.

The article is organized as follows: in Section 2 the geometry of the considered thermodiffusive composite material with periodic microstructure is illustrated, and the corresponding constitutive relations and balance equations are introduced. The developed multiscale asymptotic homogenization technique is described in Section 3, based on down-scaling relations correlating the microscopic fields to the macroscopic displacements, temperature and chemical potential. 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, averaged field equations of infinite order are obtained, and a solution scheme based on asymptotic expansion of the macroscopic displacements, temperature and chemical potential field is reported. Field equations and explicit expressions for the overall elastic and thermodiffusive constants of the equivalent first order homogeneous continuum are derived in Section 4. As just anticipated, the proposed approach is applied for studying overall properties of two-dimensional bi-phase orthotropic layered materials in Section 5. Finally, a critical discussion about the obtained results is reported together with conclusions and future perspectives in Section 6.

2 Governing equations of periodic multiphase materials in presence of thermodiffusion

Let us consider an heterogeneous composite material having periodic micro-structure and subject to stresses induced by temperature changes, mass diffusion and body forces. The two-dimensional geometry shown in Fig. 1 is assumed for the system. Considering small strains approximation, the constituent elements of the medium are modelled as a linear thermodiffusive elastic Cauchy continua. The material point is identified by position vector $\mathbf{x} = x_1\mathbf{e}_1 + x_2\mathbf{e}_2$ referred to a system of

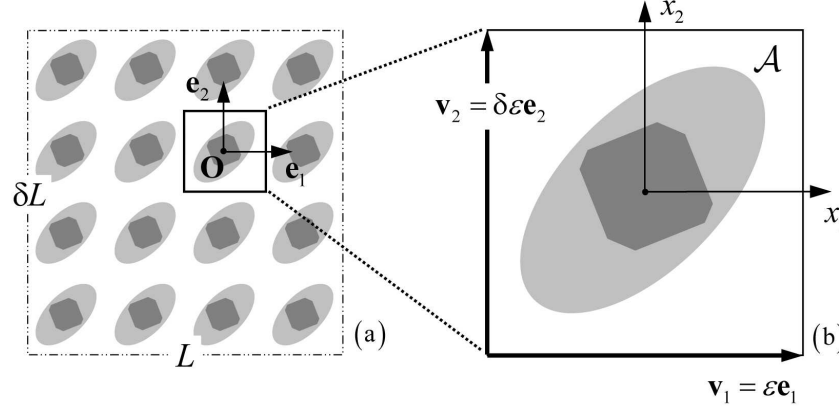


Figure 1: (a) Heterogeneous material – Periodic domain L ; (b) Periodic cell \mathcal{A} and periodicity vectors.

coordinates with origin at point O and orthogonal base $\{\mathbf{e}_1, \mathbf{e}_2\}$. The periodic cell $\mathcal{A} = [0, \varepsilon] \times [0, \delta\varepsilon]$ with characteristic size ε is illustrated in Fig. 1b. The entire periodic medium can be obtained spanning the cell \mathcal{A} by the two orthogonal vectors $\mathbf{v}_1 = d_1\mathbf{e}_1 = \varepsilon\mathbf{e}_1, \mathbf{v}_2 = d_2\mathbf{e}_2 = \delta\varepsilon\mathbf{e}_2$.

According to the periodicity of the material, \mathcal{A} is the elementary cell period of the elasticity tensor $\mathbb{C}^{(m,\varepsilon)}(\mathbf{x})$:

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

where the superscript m stands for *microscopic* field. Similarly, the heat conduction tensor $\mathbf{K}^{(m,\varepsilon)}(\mathbf{x})$ and the thermal dilatation tensor $\boldsymbol{\alpha}^{(m,\varepsilon)}(\mathbf{x})$ are defined as follows

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

and then the mass diffusion tensor $\mathbf{D}^{(m,\varepsilon)}(\mathbf{x})$ and diffusive expansion tensor $\boldsymbol{\beta}^{(m,\varepsilon)}(\mathbf{x})$ become

$$\mathbf{D}^{(m,\varepsilon)}(\mathbf{x} + \mathbf{v}_i) = \mathbf{D}^{(m,\varepsilon)}(\mathbf{x}), \quad \boldsymbol{\beta}^{(m,\varepsilon)}(\mathbf{x} + \mathbf{v}_i) = \boldsymbol{\beta}^{(m,\varepsilon)}(\mathbf{x}), \quad i = 1, 2, \quad \forall \mathbf{x} \in \mathcal{A}. \quad (3)$$

The tensors (1), (2) and (3) are commonly referred to as \mathcal{A} –periodic functions.

The system is subject to body forces $\mathbf{b}(\mathbf{x})$, heat source $r(\mathbf{x})$ and mass source $s(\mathbf{x})$ 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 the body forces, heat sources and mass sources are characterized by a period much greater than the microstructural size ε .

Following the procedure reported in Bacigalupo (2014), 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. Two distinct scales are represented by the macroscopic (slow) variables $\mathbf{x} \in \mathcal{A}$ and the microscopic (fast) variable $\boldsymbol{\xi} = \mathbf{x}/\varepsilon \in \mathcal{Q}$ (see for example Bakhvalov and Panasenko (1984); Smyshlyaev and Cherednichenko (2000) and Bacigalupo (2014)). The constitutive tensors (1), (2) and (3) are functions of the microscopic variable, whereas the body forces, heat sources and mass sources depend by the slow macroscopic variable. Consequently, the mapping of both the elasticity and thermodiffusive tensors may be defined on \mathcal{Q} as follows: $\mathbb{C}^{(m,\varepsilon)}(\mathbf{x}) = \mathbb{C}^m(\boldsymbol{\xi}) =$

\mathbf{x}/ε), $\mathbf{K}^{(m,\varepsilon)}(\mathbf{x}) = \mathbf{K}^m(\boldsymbol{\xi} = \mathbf{x}/\varepsilon)$, $\boldsymbol{\alpha}^{(m,\varepsilon)}(\mathbf{x}) = \boldsymbol{\alpha}^m(\boldsymbol{\xi} = \mathbf{x}/\varepsilon)$, $\mathbf{D}^{(m,\varepsilon)}(\mathbf{x}) = \mathbf{D}^m(\boldsymbol{\xi} = \mathbf{x}/\varepsilon)$, $\boldsymbol{\beta}^{(m,\varepsilon)}(\mathbf{x}) = \boldsymbol{\beta}^m(\boldsymbol{\xi} = \mathbf{x}/\varepsilon)$, respectively.

The relevant micro-fields are the micro-displacement $\mathbf{u}(\mathbf{x})$, the microscopic temperature $\theta(\mathbf{x}) = T(\mathbf{x}) - T_0$ (T_0 stands for the temperature of the natural state) and the microscopic chemical potential $\eta(\mathbf{x})$. The micro-stress $\boldsymbol{\sigma}(\mathbf{x})$, the microscopic heat and mass fluxes $\mathbf{q}(\mathbf{x})$ and $\mathbf{j}(\mathbf{x})$ are defined by the following constitutive relations:

$$\boldsymbol{\sigma}(\mathbf{x}) = \mathbb{C}^m \left(\frac{\mathbf{x}}{\varepsilon} \right) \boldsymbol{\varepsilon}(\mathbf{x}) - \boldsymbol{\alpha}^m \left(\frac{\mathbf{x}}{\varepsilon} \right) \theta(\mathbf{x}) - \boldsymbol{\beta}^m \left(\frac{\mathbf{x}}{\varepsilon} \right) \eta(\mathbf{x}), \quad (4)$$

$$\mathbf{q}(\mathbf{x}) = -\mathbf{K}^m \left(\frac{\mathbf{x}}{\varepsilon} \right) \nabla \theta(\mathbf{x}), \quad \mathbf{j}(\mathbf{x}) = -\mathbf{D}^m \left(\frac{\mathbf{x}}{\varepsilon} \right) \nabla \eta(\mathbf{x}), \quad (5)$$

where $\boldsymbol{\varepsilon}(\mathbf{x}) = \text{sym} \nabla \mathbf{u}(\mathbf{x})$ is the micro-strain tensor which is assumed to be zero at the fundamental state of the system.

Note that, in eqs. (5) describing the heat and mass fluxes, we confine ourselves to the essential effects and neglect coupling terms, which is an assumption generally accepted in the quasi-static theory of thermodiffusion, see for instance Nowacki (1974).

The micro-stresses (4) and the microscopic fluxes (5) satisfy the local balance equations on the domain \mathcal{A}

$$\nabla \cdot \boldsymbol{\sigma}(\mathbf{x}) + \mathbf{b}(\mathbf{x}) = \mathbf{0}, \quad \nabla \cdot \mathbf{q}(\mathbf{x}) - r(\mathbf{x}) = 0, \quad \nabla \cdot \mathbf{j}(\mathbf{x}) - s(\mathbf{x}) = 0. \quad (6)$$

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

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

$$\nabla \cdot \left(\mathbf{K}^m \left(\frac{\mathbf{x}}{\varepsilon} \right) \nabla \theta(\mathbf{x}) \right) + r(\mathbf{x}) = 0, \quad \nabla \cdot \left(\mathbf{D}^m \left(\frac{\mathbf{x}}{\varepsilon} \right) \nabla \eta(\mathbf{x}) \right) + s(\mathbf{x}) = 0. \quad (8)$$

Moreover, at the interface Σ between two different phase of the material, the microscopic fields satisfy the following interface conditions:

$$[[\mathbf{u}(\mathbf{x})]]|_{\mathbf{x} \in \Sigma} = 0, \quad \left[\left[\left(\mathbb{C}^m \left(\frac{\mathbf{x}}{\varepsilon} \right) \nabla \mathbf{u}(\mathbf{x}) - \boldsymbol{\alpha}^m \left(\frac{\mathbf{x}}{\varepsilon} \right) \theta(\mathbf{x}) - \boldsymbol{\beta}^m \left(\frac{\mathbf{x}}{\varepsilon} \right) \eta(\mathbf{x}) \right) \mathbf{n} \right] \right] |_{\mathbf{x} \in \Sigma} = 0, \quad (9)$$

$$[[\theta(\mathbf{x})]]|_{\mathbf{x} \in \Sigma} = 0, \quad \left[\left[\mathbf{K}^m \left(\frac{\mathbf{x}}{\varepsilon} \right) \nabla \theta(\mathbf{x}) \cdot \mathbf{n} \right] \right] |_{\mathbf{x} \in \Sigma} = 0, \quad (10)$$

$$[[\eta(\mathbf{x})]]|_{\mathbf{x} \in \Sigma} = 0, \quad \left[\left[\mathbf{D}^m \left(\frac{\mathbf{x}}{\varepsilon} \right) \nabla \eta(\mathbf{x}) \cdot \mathbf{n} \right] \right] |_{\mathbf{x} \in \Sigma} = 0, \quad (11)$$

where the notation $[[f]] = f^i(\Sigma) - f^j(\Sigma)$ denotes the difference between the values of a function f at the interface Σ separating the phase i from the phase j .

The micro-displacement, microscopic temperature and chemical potential may be seen in the form $\mathbf{u}(\mathbf{x}, \boldsymbol{\xi} = \mathbf{x}/\varepsilon)$, $\theta(\mathbf{x}, \boldsymbol{\xi} = \mathbf{x}/\varepsilon)$, $\eta(\mathbf{x}, \boldsymbol{\xi} = \mathbf{x}/\varepsilon)$ as functions of both the slow and the fast variable.

It is important to note that since $\mathbf{u}(\mathbf{x}, \boldsymbol{\xi})$, $\theta(\mathbf{x}, \boldsymbol{\xi})$ and $\eta(\mathbf{x}, \boldsymbol{\xi})$ are assumed to be \mathcal{Q} -periodic smoothing functions with respect to the variable \mathbf{x} , the interface conditions (9)-(11) can be expressed directly in function of the fast variable $\boldsymbol{\xi}$ (Bakhvalov and Panasenko, 1984).

The solution of microscopic field equations (7), (8) is computationally very expensive and provides too detailed results to be of practical use, so that it is convenient to replace the heterogeneous

model with an equivalent homogeneous one to obtain equations whose coefficients are not rapidly oscillating while their solutions are close to those of the original equations.

Further in the paper, assuming that the size of the microstructure ε is sufficiently small with respect to the structural size L , an equivalent classical first order thermodiffusive continuum is considered. The overall elastic moduli, thermal and diffusion expansion tensors, thermal and diffusive conduction tensors of a homogeneous continuum equivalent to periodic heterogeneous material reported in Fig. 1 are derived by means of asymptotic homogenization techniques based on the generalization of down-scaling relations. The overall elastic and thermodiffusive properties of the homogeneous continuum are expressed in terms of geometrical, mechanical, thermal and diffusive properties of the microstructure by means of an asymptotic expansion for the microscopic fields. The asymptotic expansion is performed in terms of the parameter ε that keeps the dependence on the slow variable \mathbf{x} separate from the fast one $\boldsymbol{\xi} = \mathbf{x}/\varepsilon$ such that two distinct scales are represented.

In the equivalent homogenized continuum, the macro-displacement $\mathbf{U}(\mathbf{x})$ of component U_i , the macroscopic temperature $\Theta(\mathbf{x})$ and chemical potential $\Upsilon(\mathbf{x})$ are defined at a point \mathbf{x} in the reference (\mathbf{e}_i , $i = 1, 2$). The displacement gradient is given by $\nabla \mathbf{U}(\mathbf{x}) = \frac{\partial U_i}{\partial x_j} \mathbf{e}_i \otimes \mathbf{e}_j = H_{ij} \mathbf{e}_i \otimes \mathbf{e}_j = \mathbf{H}(\mathbf{x})$, and then the macroscopic strain is $\mathbf{E}(\mathbf{x}) = \text{sym} \nabla \mathbf{U}(\mathbf{x})$. The macro-stress $\boldsymbol{\Sigma}(\mathbf{x})$ associate to $\mathbf{E}(\mathbf{x})$ are defined as $\boldsymbol{\Sigma}(\mathbf{x}) = \Sigma_{ij} \mathbf{e}_i \otimes \mathbf{e}_j$ with $\Sigma_{ij} = \Sigma_{ji}$, and the macroscopic heat and mass fluxes are respectively: $\mathbf{Q}(\mathbf{x}) = Q_i \mathbf{e}_i$ and $\mathbf{J}(\mathbf{x}) = J_i \mathbf{e}_i$.

3 Multiscale analysis and asymptotic solution of the heterogeneous problem

3.1 Down-scaling and up-scaling relations

Following the approaches developed in Bakhvalov and Panasenko (1984); Smyshlyaev and Cherednichenko (2000); Bacigalupo and Gambarotta (2014) and Bacigalupo (2014) for purely elastic problems in periodic heterogeneous media, the microscopic displacement, temperature and chemical potential fields are represented through an asymptotic expansion with respect to the parameter ε , whose terms depend on macroscopic fields and perturbation functions:

$$\begin{aligned}
u_k \left(\mathbf{x}, \boldsymbol{\xi} = \frac{\mathbf{x}}{\varepsilon} \right) &= \left[U_k(\mathbf{x}) + \sum_{l=1}^{+\infty} \varepsilon^l \sum_{|q|=l} N_{kpq}^{(l)}(\boldsymbol{\xi}) \frac{\partial^l U_p(\mathbf{x})}{\partial x_q} + \right. \\
&\quad \left. + \sum_{l=1}^{+\infty} \varepsilon^l \sum_{|q|=l-1} \left(\tilde{N}_{kq-1}^{(l)}(\boldsymbol{\xi}) \frac{\partial^{l-1} \Theta(\mathbf{x})}{\partial x_q} + \hat{N}_{kq-1}^{(l)}(\boldsymbol{\xi}) \frac{\partial^{l-1} \Upsilon(\mathbf{x})}{\partial x_q} \right) \right]_{\boldsymbol{\xi}=\mathbf{x}/\varepsilon} \\
&= U_k(\mathbf{x}) + \varepsilon \left(N_{kpq_1}^{(1)}(\boldsymbol{\xi}) \frac{\partial U_p(\mathbf{x})}{\partial x_{q_1}} + \tilde{N}_k^{(1)}(\boldsymbol{\xi}) \Theta(\mathbf{x}) + \hat{N}_k^{(1)}(\boldsymbol{\xi}) \Upsilon(\mathbf{x}) \right)_{\boldsymbol{\xi}=\mathbf{x}/\varepsilon} + \\
&\quad + \varepsilon^2 \left(N_{kpq_1q_2}^{(2)}(\boldsymbol{\xi}) \frac{\partial^2 U_p(\mathbf{x})}{\partial x_{q_1} \partial x_{q_2}} + \tilde{N}_{kq_1}^{(2)}(\boldsymbol{\xi}) \frac{\partial \Theta(\mathbf{x})}{\partial x_{q_1}} + \hat{N}_{kq_1}^{(2)}(\boldsymbol{\xi}) \frac{\partial \Upsilon(\mathbf{x})}{\partial x_{q_1}} \right)_{\boldsymbol{\xi}=\mathbf{x}/\varepsilon} + \dots,
\end{aligned} \tag{12}$$

$$\begin{aligned}
\theta\left(\mathbf{x}, \boldsymbol{\xi} = \frac{\mathbf{x}}{\varepsilon}\right) &= \left[\Theta(\mathbf{x}) + \sum_{l=1}^{+\infty} \varepsilon^l \sum_{|q|=l} \left(M_q^{(l)}(\boldsymbol{\xi}) \frac{\partial^l \Theta(\mathbf{x})}{\partial x_q} \right) \right]_{\boldsymbol{\xi}=\mathbf{x}/\varepsilon} \\
&= \Theta(\mathbf{x}) + \varepsilon \left(M_{q_1}^{(1)}(\boldsymbol{\xi}) \frac{\partial \Theta(\mathbf{x})}{\partial x_{q_1}} \right)_{\boldsymbol{\xi}=\mathbf{x}/\varepsilon} + \varepsilon^2 \left(M_{q_1 q_2}^{(2)}(\boldsymbol{\xi}) \frac{\partial^2 \Theta(\mathbf{x})}{\partial x_{q_1} \partial x_{q_2}} \right)_{\boldsymbol{\xi}=\mathbf{x}/\varepsilon} + \dots,
\end{aligned} \tag{13}$$

$$\begin{aligned}
\eta\left(\mathbf{x}, \boldsymbol{\xi} = \frac{\mathbf{x}}{\varepsilon}\right) &= \left[\Upsilon(\mathbf{x}) + \sum_{l=1}^{+\infty} \varepsilon^l \sum_{|q|=l} \left(W_q^{(l)}(\boldsymbol{\xi}) \frac{\partial^l \Upsilon(\mathbf{x})}{\partial x_q} \right) \right]_{\boldsymbol{\xi}=\mathbf{x}/\varepsilon} \\
&= \Upsilon(\mathbf{x}) + \varepsilon \left(W_{q_1}^{(1)}(\boldsymbol{\xi}) \frac{\partial \Upsilon(\mathbf{x})}{\partial x_{q_1}} \right)_{\boldsymbol{\xi}=\mathbf{x}/\varepsilon} + \varepsilon^2 \left(W_{q_1 q_2}^{(2)}(\boldsymbol{\xi}) \frac{\partial^2 \Upsilon(\mathbf{x})}{\partial x_{q_1} \partial x_{q_2}} \right)_{\boldsymbol{\xi}=\mathbf{x}/\varepsilon} + \dots.
\end{aligned} \tag{14}$$

In equations (12), (13) and (14) (commonly known as *down-scaling* relations), $q = q_1, \dots, q_l$ is a multi-index and $\partial^l(\cdot)/\partial x_q = \partial^l(\cdot)/\partial x_{q_1} \dots \partial x_{q_l}$. Due to their dependence on the slow space variable \mathbf{x} , the macroscopic fields U_k, Θ and Υ are \mathcal{L} -periodic functions. $N_{kpq}^{(l)}, M_q^{(l)}$ and $W_q^{(l)}$ are the mechanical, thermal and diffusive fluctuation functions, respectively, whereas $\tilde{N}_{kq}^{(l)}$ and $\hat{N}_{kq}^{(l)}$ denote the additional fluctuation functions corresponding to the contribution of the thermodiffusion to local displacement. All these perturbation functions depend on the fast space variable $\boldsymbol{\xi} = \mathbf{x}/\varepsilon$, and moreover, as it will be shown in Section 3.2, they are \mathcal{Q} -periodic. Similarly to the procedure reported in Smyshlyaev and Cherednichenko (2000) and Bacigalupo (2014), the mean value of the fluctuation functions is assumed to vanish on the unit cell \mathcal{Q} , this means that the following normalization conditions are satisfied:

$$\begin{aligned}
\langle N_{kpq}^{(l)} \rangle &= \frac{1}{\delta} \int_{\mathcal{Q}} N_{kpq}^{(l)}(\boldsymbol{\xi}) d\boldsymbol{\xi} = 0, \quad \langle \tilde{N}_{kq}^{(l)} \rangle = \frac{1}{\delta} \int_{\mathcal{Q}} \tilde{N}_{kq}^{(l)}(\boldsymbol{\xi}) d\boldsymbol{\xi} = 0, \quad \langle \hat{N}_{kq}^{(l)} \rangle = \frac{1}{\delta} \int_{\mathcal{Q}} \hat{N}_{kq}^{(l)}(\boldsymbol{\xi}) d\boldsymbol{\xi} = 0, \\
\langle M_q^{(l)} \rangle &= \frac{1}{\delta} \int_{\mathcal{Q}} M_q^{(l)}(\boldsymbol{\xi}) d\boldsymbol{\xi} = 0, \quad \langle W_q^{(l)} \rangle = \frac{1}{\delta} \int_{\mathcal{Q}} W_q^{(l)}(\boldsymbol{\xi}) d\boldsymbol{\xi} = 0.
\end{aligned} \tag{15}$$

Introducing a new variable $\boldsymbol{\zeta} \in \mathcal{Q}$ and a vector $\varepsilon\boldsymbol{\zeta} \in \mathcal{A}$, which represents the translations of the medium with respect to the \mathcal{L} -periodic body forces $\mathbf{b}(\mathbf{x})$, heat sources $r(\mathbf{x})$ and mass sources $s(\mathbf{x})$ (Bacigalupo and Gambarotta, 2014), it can be shown that any \mathcal{Q} -periodic function $g(\boldsymbol{\xi} + \boldsymbol{\zeta})$ satisfies the following invariance property:

$$\langle g(\boldsymbol{\xi} + \boldsymbol{\zeta}) \rangle = \frac{1}{\delta} \int_{\mathcal{Q}} g(\boldsymbol{\xi} + \boldsymbol{\zeta}) d\boldsymbol{\zeta} = \frac{1}{\delta} \int_{\mathcal{Q}} g(\boldsymbol{\xi} + \boldsymbol{\zeta}) d\boldsymbol{\xi}. \tag{16}$$

According to the invariance property (16) and to the normalization conditions (15), the macroscopic fields can be defined as the mean values of the microscopic quantities (12), (13) and (14) evaluated on the unit cell \mathcal{Q} :

$$U_k(\mathbf{x}) \doteq \left\langle u_k \left(\mathbf{x}, \frac{\mathbf{x}}{\varepsilon} + \boldsymbol{\zeta} \right) \right\rangle, \quad \Theta(\mathbf{x}) \doteq \left\langle \theta \left(\mathbf{x}, \frac{\mathbf{x}}{\varepsilon} + \boldsymbol{\zeta} \right) \right\rangle, \quad \Upsilon(\mathbf{x}) \doteq \left\langle \eta \left(\mathbf{x}, \frac{\mathbf{x}}{\varepsilon} + \boldsymbol{\zeta} \right) \right\rangle, \tag{17}$$

Expressions (17) are commonly known as *up-scaling* relations. More details regarding the structure of the down-scaling relations (12), (13) and (14) are provided in Appendix D.

3.2 First-order asymptotic analysis and derivation of the corresponding first-order cell problems

In order to derive exact expressions for the fluctuation functions affecting the behavior of the microscopic fields u_k, θ, η , the *down-scaling* relations (12), (13) and (14) are substituted into the microscopic field equations (7), (8). Remembering the property $\frac{\partial}{\partial x_j} f(\mathbf{x}, \boldsymbol{\xi} = \frac{\mathbf{x}}{\varepsilon}) = \left(\frac{\partial f}{\partial x_j} + \frac{1}{\varepsilon} \frac{\partial f}{\partial \xi_j} \right)_{\boldsymbol{\xi}=\mathbf{x}/\varepsilon} = \left(\frac{\partial f}{\partial x_j} + \frac{f_{,j}}{\varepsilon} \right)_{\boldsymbol{\xi}=\mathbf{x}/\varepsilon}$, equation (7) become to the first order approximation

$$\varepsilon^{-1} \left\{ \left[\left(C_{ijkl}^\varepsilon N_{kpq_1, l}^{(1)} \right)_{,j} + C_{ijpq_1, j}^\varepsilon \right] H_{pq_1}(\mathbf{x}) + \left[\left(C_{ijkl}^\varepsilon \tilde{N}_{k, l}^{(1)} \right)_{,j} - \alpha_{ij, j}^\varepsilon \right] \Theta(\mathbf{x}) + \left[\left(C_{ijkl}^\varepsilon \hat{N}_{k, l}^{(1)} \right)_{,j} - \beta_{ij, j}^\varepsilon \right] \Upsilon(\mathbf{x}) \right\} + \dots + b_i(\mathbf{x}) = 0, \quad i = 1, 2, \quad (18)$$

where $H_{pq_1} = \partial U_p / \partial x_{q_1}$ are the components of the macroscopic displacement gradient tensor previously defined. Equations (8) assume the following form

$$\varepsilon^{-1} \left[\left(K_{ij}^\varepsilon M_{q_1, j}^{(1)} \right)_{,i} + K_{iq_1, i}^\varepsilon \right] \frac{\partial \Theta}{\partial x_{q_1}} + \dots + r(\mathbf{x}) = 0, \quad (19)$$

$$\varepsilon^{-1} \left[\left(D_{ik}^\varepsilon W_{q_1, j}^{(1)} \right)_{,i} + D_{iq_1, i}^\varepsilon \right] \frac{\partial \Upsilon}{\partial x_{q_1}} + \dots + s(\mathbf{x}) = 0. \quad (20)$$

In order to transform the field equation (18), (19) and (20) in a PDEs system with constant coefficients, in which the unknowns are the macroscopic quantities $U_k(\mathbf{x})$, $\Theta(\mathbf{x})$ and $\Upsilon(\mathbf{x})$, the fluctuation functions have to satisfy non-homogeneous equations (*first-order cell problems*) reported below.

At the order ε^{-1} from the equation (18) we derive:

$$\left(C_{ijkl}^\varepsilon N_{kpq_1, l}^{(1)} \right)_{,j} + C_{ijpq_1, j}^\varepsilon = n_{ipq_1}^{(1)}, \quad \left(C_{ijkl}^\varepsilon \tilde{N}_{k, l}^{(1)} \right)_{,j} - \alpha_{ij, j}^\varepsilon = \tilde{n}_i^{(1)}, \quad \left(C_{ijkl}^\varepsilon \hat{N}_{k, l}^{(1)} \right)_{,j} - \beta_{ij, j}^\varepsilon = \hat{n}_i^{(1)}, \quad (21)$$

whereas from thermodiffusion equations (19) and (20) we obtain:

$$\left(K_{ij}^\varepsilon M_{q_1, j}^{(1)} \right)_{,i} + K_{iq_1, i}^\varepsilon = m_{q_1}^{(1)}, \quad \left(D_{ij}^\varepsilon W_{q_1, j}^{(1)} \right)_{,i} + D_{iq_1, i}^\varepsilon = w_{q_1}^{(1)}, \quad (22)$$

where:

$$n_{ipq_1}^{(1)} = \langle C_{ijpq_1, j}^\varepsilon \rangle = 0, \quad \tilde{n}_i^{(1)} = -\langle \alpha_{ij, j}^\varepsilon \rangle = 0, \quad \hat{n}_i^{(1)} = -\langle \beta_{ij, j}^\varepsilon \rangle = 0, \\ m_{q_1}^{(1)} = \langle K_{iq_1, i}^\varepsilon \rangle = 0, \quad w_{q_1}^{(1)} = \langle D_{iq_1, i}^\varepsilon \rangle = 0. \quad (23)$$

The properties (23) are consequence of the \mathcal{Q} -periodicity of the components $C_{ijpq_1}^\varepsilon, \alpha_{ij}^\varepsilon, \beta_{ij}^\varepsilon, K_{iq_1}^\varepsilon$ and $D_{iq_1}^\varepsilon$. Note that in equations (18)–(23) the derivatives should be understood in the generalized sense.

The perturbation functions characterizing the *down-scaling* relations (12), (13), and (14) are obtained by the solution of the previously defined cells problems, derived by imposing the normalization conditions (15).

4 Homogenized thermodiffusive Cauchy continuum: field equations and overall properties

The field equations of the first order homogeneous continuum can be obtained by the zero order terms (equations (63) and (64)) of the sequence of PDEs derived applying the asymptotic analysis to the averaged field equation, see Appendix A. This implies that the macroscopic displacement, temperature and chemical potential are approximated as follows:

$$U_p(\mathbf{x}) \approx U_p^{(0)}(\mathbf{x}), \quad \Theta(\mathbf{x}) \approx \Theta^{(0)}(\mathbf{x}), \quad \Upsilon(\mathbf{x}) \approx \Upsilon^{(0)}(\mathbf{x}). \quad (24)$$

Alternatively, the field equations of the equivalent Cauchy continuum can be derived considering only the terms of order ε^0 in the equations (59), (60) and (61).

The field equations of an homogeneous first order continuum in presence of thermodiffusion are given by

$$C_{iq_1pq_2} \frac{\partial^2 U_p}{\partial x_{q_1} \partial x_{q_2}} - \alpha_{iq_1} \frac{\partial \Theta}{\partial x_{q_1}} - \beta_{iq_1} \frac{\partial \Upsilon}{\partial x_{q_1}} + b_i = 0, \quad (25)$$

$$K_{q_1q_2} \frac{\partial^2 \Theta}{\partial x_{q_1} \partial x_{q_2}} + r = 0, \quad D_{q_1q_2} \frac{\partial^2 \Upsilon}{\partial x_{q_1} \partial x_{q_2}} + s = 0, \quad (26)$$

where $C_{iq_1pq_2}$ are the components of the overall elastic tensor, α_{iq_1} and β_{iq_1} are respectively the components of the overall thermal dilatation and diffusive expansion tensors, $K_{q_1q_2}$ denotes the components of the overall heat conduction tensor and $D_{q_1q_2}$ represents the components of the overall mass diffusion tensor. Remembering the approximation (24), the macroscopic field equations (25)–(26) can be compared to the zero order terms of the averaged field equation (63) and (64) for determining the overall properties of the thermodiffusive Cauchy continuum. In order to relate the coefficients $n_{ipq_1q_2}^{(2)}$, $\tilde{n}_{iq_1}^{(2)}$, $\hat{n}_{iq_1}^{(2)}$, $m_{q_1q_2}^{(2)}$, $w_{q_1q_2}^{(2)}$ contained in the equations (63) and (64) to the overall elastic and thermodiffusive constants of the media $C_{iq_1pq_2}$, α_{iq_1} , β_{iq_1} , $K_{q_1q_2}$, $D_{q_1q_2}$, the symmetries of the tensors of components $n_{ipq_1q_2}^{(2)}$, $\tilde{n}_{iq_1}^{(2)}$, $\hat{n}_{iq_1}^{(2)}$, $m_{q_1q_2}^{(2)}$, $w_{q_1q_2}^{(2)}$, and the ellipticity of the field equations (63) and (64) are required. A demonstration of these properties is reported in Appendix C. As a consequence of these properties, it can be observed that: $n_{ipq_1q_2}^{(2)} = \frac{1}{2}(C_{iq_1pq_2} + C_{iq_2pq_1})$, $\tilde{n}_{iq_1}^{(2)} = \alpha_{iq_1}$, $\hat{n}_{iq_1}^{(2)} = \beta_{iq_1}$, $m_{q_1q_2}^{(2)} = K_{q_1q_2}$ and $w_{q_1q_2}^{(2)} = D_{q_1q_2}$. In particular, comparing the field equation (25) to (63), and remembering the relationship between $n_{ipq_1q_2}^{(2)}$ and $C_{iq_1pq_2}$, it is easy to note that due to the repetition of the indexes q_1 and q_2 : $C_{iq_1pq_2} \frac{\partial^2 U_p}{\partial x_{q_1} \partial x_{q_2}} = n_{ipq_1q_2}^{(2)} \frac{\partial^2 U_p}{\partial x_{q_1} \partial x_{q_2}} = \frac{1}{2}(C_{iq_1pq_2} + C_{iq_2pq_1}) \frac{\partial^2 U_p}{\partial x_{q_1} \partial x_{q_2}}$.

The overall elastic and thermodiffusive tensors, obtained in terms of fluctuation functions, and the components of microscopic elastic and thermodiffusive tensors, take the form (see Appendix A for details):

$$\begin{aligned} C_{iq_1pq_2} &= \frac{1}{4} \left\langle C_{rjkl}^\varepsilon \left(N_{riq_1,j}^{(1)} + \delta_{ri} \delta_{jq_1} + N_{rq_1i,j}^{(1)} + \delta_{rq_1} \delta_{ij} \right) \left(N_{kpq_2,l}^{(1)} + \delta_{kp} \delta_{q_2,l} + N_{kq_2p,l}^{(1)} + \delta_{kq_2} \delta_{lp} \right) \right\rangle \\ \alpha_{iq_1} &= \left\langle C_{iq_1kl}^\varepsilon \tilde{N}_{k,l}^{(1)} - \alpha_{iq_1}^\varepsilon \right\rangle, \quad \beta_{iq_1} = \left\langle C_{iq_1kl}^\varepsilon \hat{N}_{k,l}^{(1)} - \beta_{iq_1}^\varepsilon \right\rangle, \\ K_{q_1q_2} &= \left\langle K_{ij}^\varepsilon (M_{q_1,j}^{(1)} + \delta_{jq_1})(M_{q_2,i}^{(1)} + \delta_{iq_2}) \right\rangle, \quad D_{q_1q_2} = \left\langle D_{ij}^\varepsilon (W_{q_1,j}^{(1)} + \delta_{jq_1})(W_{q_2,i}^{(1)} + \delta_{iq_2}) \right\rangle. \end{aligned} \quad (27)$$

The components $C_{iq_1pq_2}$, $K_{q_1q_2}$ and $D_{q_1q_2}$ of the overall constitutive tensors of the material coincide with those derived by asymptotic homogenization techniques applied to uncoupled static

elastic (Bakhvalov and Panasenko, 1984; Smyshlyaev and Cherednichenko, 2000; Bacigalupo, 2014) and heat conduction problems (Zhang et al., 2007) in media with periodic microstructures. The components α_{iq_1} and β_{iq_1} of the coupling thermodiffusive tensors have been obtained by means of a consistent generalization of the down-scaling relations (12) (13) and (14). These expressions relate the microscopic displacement field to the macroscopic displacements, temperature, chemical potential and their higher order gradients.

5 Illustrative example: homogenization of bi-phase orthotropic layered materials in presence of thermodiffusion

The general results obtained are now applied to the case of a bi-phase layered material in presence of thermodiffusion. Exact analytical expressions for the overall elastic and thermodiffusive constants are derived. Considering a two-dimensional infinite thermodiffusive medium subject to periodic body forces, heat and/or mass sources, the solution obtained applying the proposed homogenized model is compared with the results provided by the analysis of the corresponding heterogeneous problem.

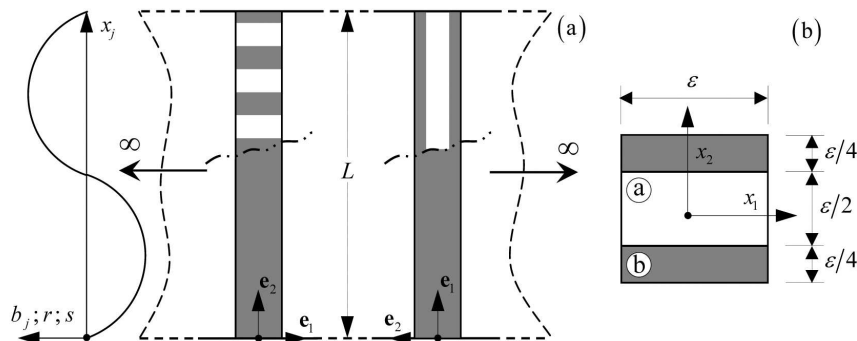


Figure 2: (a) Heterogeneous and homogenized models with \mathcal{L} -periodic body force b_j , heat sources $r(x_j)$ and mass sources $s(x_j)$; (b) Periodic cell and constituents: bi-phase layered material.

5.1 Perturbation functions and overall constitutive constants: exact analytical expressions

Let us consider a layered body obtained as an unbounded d_2 -periodic arrangement of two different layers having thickness a and b , where $d_2 = \varepsilon = a + b$ and $\zeta = a/b$ are defined. The phases are assumed homogeneous and orthotropic, with an orthotropic axis coincident with the layering direction \mathbf{e}_1 , the geometry of the system is shown in Fig. 2. The orthotropic symmetry is assumed for both the elastic and thermodiffusive tensors. The micro-fluctuation functions $N_{riq_1}^{(1)}$, $\tilde{N}_k^{(1)}$, $\hat{N}_k^{(1)}$, $M_{q_1}^{(1)}$ and $W_{q_1}^{(1)}$ are analytically obtained through the solution of the cell problems formulated in Section 3.2 (see equations (21) and (22) and conditions (23)). Due to the particular properties of symmetry of the microstructure, these functions depend only on the fast variable ξ_2 . This variable

is perpendicular to the layering direction \mathbf{e}_1 (see Fig. 2). The non-vanishing micro-fluctuation functions $N_{riq_1}^{(1)}$, $\tilde{N}_k^{(1)}$ and $\hat{N}_k^{(1)}$, obtained by solving the cell problem of order ε^{-1} (21) are:

$$\begin{aligned} N_{211}^{(1)-a} &= \frac{C_{1122}^b - C_{1122}^a}{C_{2222}^a - \zeta C_{2222}^b} \xi_2^a; & N_{211}^{(1)-b} &= \zeta \frac{C_{1122}^a - C_{1122}^b}{C_{2222}^a - \zeta C_{2222}^b} \xi_2^b; \\ N_{222}^{(1)-a} &= \frac{C_{2222}^b - C_{2222}^a}{C_{2222}^a - \zeta C_{2222}^b} \xi_2^a; & N_{211}^{(1)-b} &= \zeta \frac{C_{1122}^a - C_{1122}^b}{C_{2222}^a - \zeta C_{2222}^b} \xi_2^b; \\ N_{112}^{(1)-a} &= N_{121}^{(1)-a} = \frac{C_{1212}^b - C_{1212}^a}{C_{1212}^a - \zeta C_{1212}^b} \xi_2^a; & N_{112}^{(1)-b} &= N_{121}^{(1)-b} = \zeta \frac{C_{1212}^a - C_{1212}^b}{C_{1212}^a - \zeta C_{1212}^b} \xi_2^b; \end{aligned} \quad (28)$$

$$\tilde{N}_2^{(1)-a} = -\frac{\alpha_{22}^b - \alpha_{22}^a}{C_{2222}^a + \zeta C_{2222}^b} \xi_2^a; \quad \tilde{N}_2^{(1)-b} = \zeta \frac{\alpha_{22}^b - \alpha_{22}^a}{C_{2222}^a + \zeta C_{2222}^b} \xi_2^b; \quad (29)$$

$$\hat{N}_2^{(1)-a} = -\frac{\beta_{22}^b - \beta_{22}^a}{C_{2222}^a + \zeta C_{2222}^b} \xi_2^a; \quad \hat{N}_2^{(1)-b} = \zeta \frac{\beta_{22}^b - \beta_{22}^a}{C_{2222}^a + \zeta C_{2222}^b} \xi_2^b; \quad (30)$$

where $\xi_2^a \in \left[-\frac{\zeta}{2(\zeta+1)}, \frac{\zeta}{2(\zeta+1)}\right]$ and $\xi_2^b \in \left[-\frac{1}{2(\zeta+1)}, \frac{1}{2(\zeta+1)}\right]$ are non-dimensional vertical coordinates centered in each layer. The non-vanishing fluctuation functions associate with the thermodiffusion equations, derived by the solution of the cell problems of order ε^{-1} (22) are:

$$M_2^{(1)-a} = -\frac{K_{22}^a - K_{22}^b}{K_{22}^a - \zeta K_{22}^b} \xi_2^a; \quad M_2^{(1)-b} = \zeta \frac{K_{22}^a - K_{22}^b}{K_{22}^a - \zeta K_{22}^b} \xi_2^b; \quad (31)$$

$$W_2^{(1)-a} = -\frac{D_{22}^a - D_{22}^b}{D_{22}^a - \zeta D_{22}^b} \xi_2^a; \quad W_2^{(1)-b} = \zeta \frac{D_{22}^a - D_{22}^b}{D_{22}^a - \zeta D_{22}^b} \xi_2^b. \quad (32)$$

Note that the superscripts a, b denote that the elastic and thermodiffusive constants are referred respectively to the phases a and b .

In order to derive the overall elastic and thermodiffusive constants corresponding to a first order equivalent continuum, the fluctuation functions (28), (29), (30), (31) and (32) are used into expressions (27). The components of the overall elastic tensor $C_{iq_1pq_2}$ take the form:

$$C_{1111} = \frac{\zeta^2 C_{1111}^a C_{2222}^b + \zeta (C_{1111}^b C_{2222}^b - (C_{1122}^a)^2 + 2C_{1122}^a C_{1122}^b - (C_{1122}^b)^2 + C_{1111}^a C_{2222}^a) + C_{1111}^b C_{2222}^a}{(\zeta + 1)(C_{2222}^a + \zeta C_{2222}^b)};$$

$$C_{2222} = \frac{(\zeta + 1)C_{2222}^a C_{2222}^b}{C_{2222}^a + \zeta C_{2222}^b}, \quad C_{1212} = \frac{(\zeta + 1)C_{1212}^a C_{1212}^b}{C_{1212}^a + \zeta C_{1212}^b}, \quad C_{1122} = \frac{C_{1122}^b C_{2222}^a + \zeta C_{1122}^a C_{2222}^b}{C_{2222}^a + \zeta C_{2222}^b}. \quad (33)$$

The non-vanishing components of the thermal dilatation tensor α_{iq_1} and diffusive expansion tensor β_{iq_1} are respectively given by

$$\begin{aligned} \alpha_{11} &= -\frac{\zeta (C_{1122}^b \alpha_{22}^b - C_{1122}^b \alpha_{22}^a - C_{2222}^b \alpha_{11}^b - C_{1122}^a \alpha_{22}^b + C_{1122}^a \alpha_{22}^a - C_{2222}^a \alpha_{11}^a) - \zeta^2 C_{2222}^b \alpha_{11}^a - C_{2222}^a \alpha_{11}^b}{(\zeta + 1)(C_{2222}^a + \zeta C_{2222}^b)}; \\ \alpha_{22} &= \frac{\zeta C_{2222}^b \alpha_{22}^a + \alpha_{22}^b C_{2222}^a}{C_{2222}^a + \zeta C_{2222}^b}; \end{aligned} \quad (34)$$

$$\beta_{11} = -\frac{\zeta(C_{1122}^b\beta_{22}^b - C_{1122}^b\beta_{22}^a - C_{2222}^b\beta_{11}^b - C_{1122}^a\beta_{22}^b + C_{1122}^a\beta_{22}^a - C_{2222}^a\beta_{11}^a) - \zeta^2 C_{2222}^b\beta_{11}^a - C_{2222}^a\beta_{11}^b}{(\zeta + 1)(C_{2222}^a + \zeta C_{2222}^b)},$$

$$\beta_{22} = \frac{\zeta C_{2222}^b\beta_{22}^a + \beta_{22}^b C_{2222}^a}{C_{2222}^a + \zeta C_{2222}^b}. \quad (35)$$

The non-vanishing components of the heat conduction tensor K_{iq_1} and mass diffusion tensor D_{iq_1} take the form

$$K_{11} = \frac{K_{11}^b + \zeta K_{11}^a}{\zeta + 1}, \quad K_{22} = \frac{(\zeta + 1)K_{22}^a K_{22}^b}{K_{22}^a + \zeta K_{22}^b}; \quad (36)$$

$$D_{11} = \frac{D_{11}^b + \zeta D_{11}^a}{\zeta + 1}, \quad D_{22} = \frac{(\zeta + 1)D_{22}^a D_{22}^b}{D_{22}^a + \zeta D_{22}^b}. \quad (37)$$

Considering the case of isotropic phases, the components of the elasticity tensor become $C_{1111}^\varsigma = C_{2222}^\varsigma = \frac{\tilde{E}_\varsigma}{1-\tilde{\nu}_\varsigma^2}$, $C_{1122}^\varsigma = \frac{\tilde{\nu}_\varsigma \tilde{E}_\varsigma}{1-\tilde{\nu}_\varsigma^2}$, $C_{1212}^\varsigma = \frac{\tilde{E}_\varsigma}{2(1+\tilde{\nu}_\varsigma)}$, (with $\varsigma = a, b$), where for plane-strain: $\tilde{E}_\varsigma = \frac{E_\varsigma}{1-\nu_\varsigma^2}$, $\tilde{\nu}_\varsigma = \frac{\nu_\varsigma}{1-\nu_\varsigma}$, whereas for plane-stress: $\tilde{E}_\varsigma = E_\varsigma$, $\tilde{\nu}_\varsigma = \nu_\varsigma$, being E_ς the Young's modulus and ν_ς the Poisson's ratio, respectively. The components of the thermal dilatation and diffusive expansion tensors take respectively the forms: $\alpha_{11}^\varsigma = \alpha_{22}^\varsigma = \alpha^\varsigma$, $\beta_{11}^\varsigma = \beta_{22}^\varsigma = \beta^\varsigma$ (note that the coefficients α^ς and β^ς can be expressed in terms of the linear isotropic thermal and diffusive expansion coefficients and the elastic moduli (Nowacki, 1974, 1986)). The components of the heat conduction and mass diffusion tensors finally become $K_{11}^\varsigma = K_{22}^\varsigma = K^\varsigma$ and $D_{11}^\varsigma = D_{22}^\varsigma = D^\varsigma$. The overall elastic and thermodiffusive constants for the case of isotropic phases are reported in Appendix C.

By an asymptotic expansion of the constants (33), (34), (35), (36) and (37) in terms of the concentration of the two constituents phases (not reported here for conciseness), it can be easily shown that, if the concentration of the phase a vanishes, the overall elastic and thermodiffusive constants of the bi-phase layered material tend to the values corresponding to phase b . Conversely, if the concentration of the phase a tends to one, the same expressions tend to the elastic and thermodiffusive constants of the phase a .

In order to simplify the required computations, for the illustrative examples both the phases are assumed to be isotropic, and then the overall elastic and thermodiffusive constants reported in Appendix C are used. These constants can be represented in the non-dimensional form:

$$\tilde{C}_{iq_1 pq_2}(\rho_C, \zeta, \tilde{\nu}_a, \tilde{\nu}_b) = \frac{C_{iq_1 pq_2}}{\tilde{C}_{iq_1 pq_2}}, \quad \tilde{\alpha}_{iq_1}(\rho_C, \rho_\alpha, \zeta, \tilde{\nu}_a, \tilde{\nu}_b) = \frac{\alpha_{iq_1}}{\tilde{\alpha}_{iq_1}}, \quad \tilde{\beta}_{iq_1}(\rho_C, \rho_\beta, \zeta, \tilde{\nu}_a, \tilde{\nu}_b) = \frac{\beta_{iq_1}}{\tilde{\beta}_{iq_1}},$$

$$\tilde{K}_{iq_1}(\rho_K, \zeta) = \frac{K_{iq_1}}{\tilde{K}_{iq_1}}, \quad \tilde{D}_{iq_1}(\rho_D, \zeta) = \frac{D_{iq_1}}{\tilde{D}_{iq_1}}, \quad (38)$$

where $\rho_C = \tilde{E}_a/\tilde{E}_b$, $\rho_\alpha = \tilde{\alpha}^a/\tilde{\alpha}^b$, $\rho_\beta = \tilde{\beta}^a/\tilde{\beta}^b$, $\rho_K = \tilde{K}^a/\tilde{K}^b$, $\rho_D = \tilde{D}^a/\tilde{D}^b$, and $\tilde{C}_{iq_1 pq_2} = (C_{iq_1 pq_2}^a + C_{iq_1 pq_2}^b)/2$, $\tilde{\alpha}_{iq_1} = (\alpha_{iq_1}^a + \alpha_{iq_1}^b)/2$, $\tilde{\beta}_{iq_1} = (\beta_{iq_1}^a + \beta_{iq_1}^b)/2$, $\tilde{K}_{iq_1} = (K_{iq_1}^a + K_{iq_1}^b)/2$, $\tilde{D}_{iq_1} = (D_{iq_1}^a + D_{iq_1}^b)/2$. It is important to note that if the Poisson's coefficients of the two phases are identical (i.e. $\nu_a = \nu_b$), the non-dimensional overall elastic and thermodiffusive constants (38) possess the following property:

$$\tilde{C}_{iq_1 pq_2}(\rho_C, \zeta, \tilde{\nu}) = \tilde{C}_{iq_1 pq_2}(\rho_C^{-1}, \zeta^{-1}, \tilde{\nu}), \quad \tilde{\alpha}_{iq_1}(\rho_C, \rho_\alpha, \zeta, \tilde{\nu}) = \tilde{\alpha}_{iq_1}(\rho_C^{-1}, \rho_\alpha^{-1}, \zeta^{-1}, \tilde{\nu}),$$

$$\tilde{\beta}_{iq_1}(\rho_C, \rho_\beta, \zeta, \tilde{\nu}) = \tilde{\beta}_{iq_1}(\rho_C^{-1}, \rho_\beta^{-1}, \zeta^{-1}, \tilde{\nu}), \quad \tilde{K}_{iq_1}(\rho_K, \zeta) = \tilde{K}_{iq_1}(\rho_K^{-1}, \zeta^{-1}),$$

$$\tilde{D}_{iq_1}(\rho_K, \zeta) = \tilde{D}_{iq_1}(\rho_K^{-1}, \zeta^{-1}). \quad (39)$$

The variation of the normalized components of the overall elasticity tensor \tilde{C}_{1111} and \tilde{C}_{2222} with the ratio ρ_C is reported in Figs. 3/(a) and 4/(a), respectively. The same value of the Poisson's coefficient $\tilde{\nu} = 0.3$ has been assumed for both the phases, and several values of the non-dimensional geometrical parameter ζ has been considered for the computations. It can be observed that for $\rho_C = 1$, corresponding to the case of two isotropic phases having identical elastic properties, the non-dimensional components of the overall elastic tensor assume the value $\tilde{C}_{iq_1pq_2} = 1$ (i. e. $C_{iq_1pq_2}^a = C_{iq_1pq_2}^b$). In Figs. 3/(b) and 4/(b) the components \tilde{C}_{1111} and \tilde{C}_{2222} are plotted as functions of ζ for different values of ρ_C considering the fixed Poisson's coefficient $\tilde{\nu} = 0.3$ identical for both the phases. For $\zeta \rightarrow 0$, the thickness of the phase *a* vanishes. Consequently, the values of the overall elastic constants tends to those of the phase *b*: $C_{iq_1pq_2} = C_{iq_1pq_2}^b$, and the limit values assumed by the normalized components of the elastic tensor reported in the figures are $\tilde{C}_{iq_1pq_2} = 2/(1 + \rho_C)$. Conversely, for $\zeta \rightarrow +\infty$ the thickness of the phase *b* tends to zero, and then $C_{iq_1pq_2} = C_{iq_1pq_2}^a$ and the non-dimensional constants plotted in Figs. 3/(b)-4/(b) assume the limit values $\tilde{C}_{iq_1pq_2} = 2\rho_C/(1 + \rho_C)$. Results (not reported here) show that the normalized components \tilde{C}_{1212} and \tilde{C}_{1122} have a behaviour very similar to that of the component \tilde{C}_{2222} .

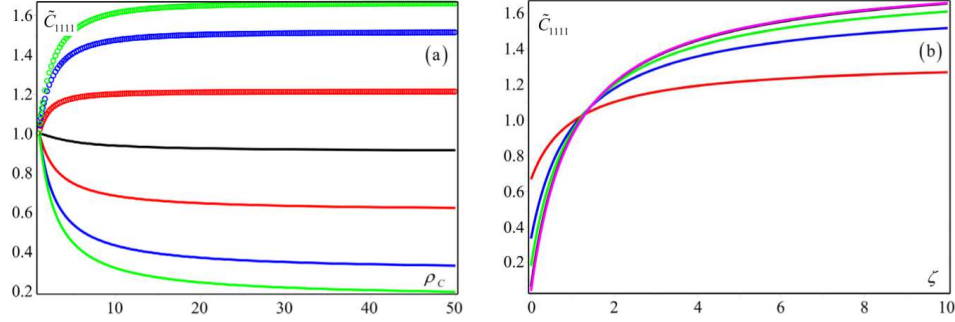


Figure 3: (a) Dimensionless constant \tilde{C}_{1111} vs. the ratio ρ_C for $\tilde{\nu}_a = \tilde{\nu}_b = 0.3$ and for different values of the geometric ratio ζ : $\zeta = 1/10$ green line, $\zeta = 1/5$ blue line, $\zeta = 1/2$ red line, $\zeta = 1/1$ black line, $\zeta = 2$ red points, $\zeta = 5$ blue points, $\zeta = 10$ green points. (b) Dimensionless constant \tilde{C}_{1111} vs. the geometric ratio ζ for $\tilde{\nu}_a = \tilde{\nu}_b = 0.3$ and for different values of the ratio ρ_C : $\rho_C = 2$ red line, $\rho_C = 5$ blue line, $\rho_C = 10$ green line, $\rho_C = 30$ black line, $\rho_C = 50$ violet line.

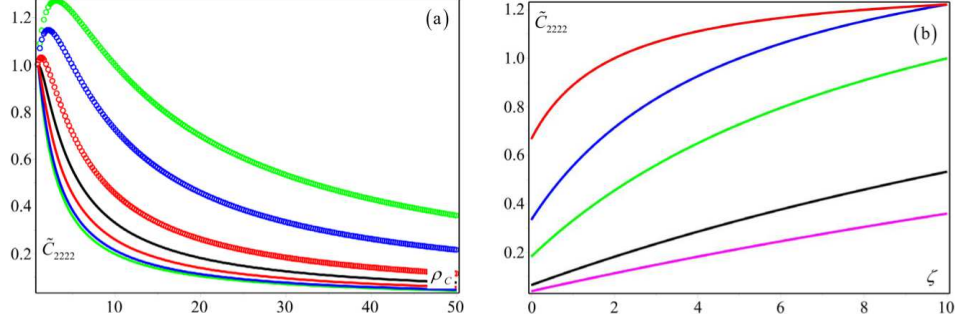


Figure 4: (a) Dimensionless constant \tilde{C}_{2222} vs. the ratio ρ_C for $\tilde{\nu}_a = \tilde{\nu}_b = 0.3$ and for different values of the geometric ratio ζ : $\zeta = 1/10$ green line, $\zeta = 1/5$ blue line, $\zeta = 1/2$ red line, $\zeta = 1$ black line, $\zeta = 2$ red points, $\zeta = 5$ blue points, $\zeta = 10$ green points. (b) Dimensionless constant \tilde{C}_{2222} vs. the geometric ratio ζ for $\tilde{\nu}_a = \tilde{\nu}_b = 0.3$ and for different values of the ratio ρ_C : $\rho_C = 2$ red line, $\rho_C = 5$ blue line, $\rho_C = 10$ green line, $\rho_C = 30$ black line, $\rho_C = 50$ violet line.

The three-dimensional plots reported in Fig. 5 show the variation of the normalized components of the overall thermal dilatation tensor $\tilde{\alpha}_{11}$ and $\tilde{\alpha}_{22}$ as functions of ρ_c and ρ_α , assuming $\tilde{\nu} = 0.3$ for both the phases and $\zeta = 1$. In Figs. 6/(a) and 7/(a) the variation of $\tilde{\alpha}_{11}$ and $\tilde{\alpha}_{22}$ with the non-dimensional ratio ρ_C is reported for several values of ζ assuming $\tilde{\nu}_a = \tilde{\nu}_b = \tilde{\nu} = 0.3$ and $\rho_\alpha = 2$. For $\rho_C = 1$, corresponding to the case of two isotropic phases with identical elastic constants but different thermal dilatation properties, the normalized components of the overall thermal dilatation tensor tend to the values $\tilde{\alpha}_{iq_1} = 2(\zeta\rho_\alpha + 1)/[(\rho_\alpha + 1)(\zeta + 1)]$ (i.e. $\alpha_{iq_1} = (\alpha_{iq_1}^a \zeta + \alpha_{iq_1}^b)/(\zeta + 1)$). In the case where $\rho_C = 1$ and also $\rho_\alpha = 1$, both the elastic and thermal dilatation tensors of the two phases are identical, and then $\tilde{\alpha}_{iq_1} = 1$. In Figs. 6/(b) and 7/(b) the same constants $\tilde{\alpha}_{11}$ and $\tilde{\alpha}_{22}$ are plotted as functions of ζ for $\tilde{\nu} = 0.3$, $\rho_\alpha = 2$ and several different values of ρ_C . For $\zeta \rightarrow 0$, the thickness for the phase a vanishes, and the elements of the overall thermal dilatation tensor tends to those of the phase b (i.e. $\alpha_{iq_1} = \alpha_{iq_1}^b$). As it can be observed in the figures, in this case the normalized constants tend to a limit value which is the same for any value of ρ_C (i.e. $\tilde{\alpha}_{iq_1} = 2/(1 + \rho_\alpha)$). This value can be easily derived by using expressions for α_{11} and α_{22} reported in Appendix C. Conversely, for $\zeta \rightarrow +\infty$, the thickness of the layer b tends to zero, the effective thermal dilatation constants tend to those of the phase a (i.e. $\alpha_{iq_1} = \alpha_{iq_1}^a$) and the normalized components $\tilde{\alpha}_{11}$ and $\tilde{\alpha}_{22}$ reported in Figs. 6/(b) and 7/(b) assume the values $\tilde{\alpha}_{iq_1} = 2\rho_\alpha/(1 + \rho_\alpha)$. The properties of the normalized elements of the overall diffusive expansion tensor $\tilde{\beta}_{11}$ and $\tilde{\beta}_{22}$ are similar to those of $\tilde{\alpha}_{11}$ and $\tilde{\alpha}_{22}$, and can be easily studied substituting the non-dimensional ratio ρ_α with ρ_β .

The variation of the normalized components of the overall heat conduction tensor \tilde{K}_{11} and \tilde{K}_{22} with the non-dimensional ratio ρ_K are shown in Figs. 8/(a) and 9/(a). Several values of ζ have been assumed for the computations. It can be observed that for $\rho_K = 1$, we have $\tilde{K}_{iq_1} = 1$. This is due to the fact that the value $\rho_K = 1$ corresponds to the case where the heat conduction of the two phases are identical, and then $K_{iq_1}^a = K_{iq_1}^b$. In Figs. 8/(a) and 9/(b) the same non-dimensional components \tilde{K}_{11} and \tilde{K}_{22} are reported as functions of ζ for different values of ρ_K . As it is shown by these figures, for $\zeta \rightarrow 0$, \tilde{K}_{11} and \tilde{K}_{22} tends to a finite value depending on ρ_K . This limit correspond to the case of vanishing thickness of the layer a , where $K_{iq_1} = K_{iq_1}^b$, and then

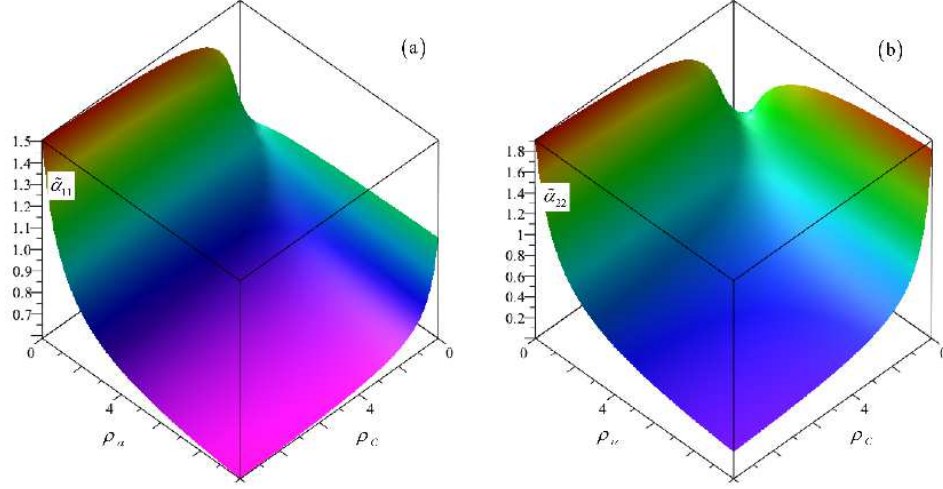


Figure 5: Dimensionless component $\tilde{\alpha}_{11}$ (a), $\tilde{\alpha}_{22}$ (b) vs. the ratios ρ_C and ρ_α for $\tilde{\nu}_a = \tilde{\nu}_b = 0.3$ and $\zeta = 1/2$.

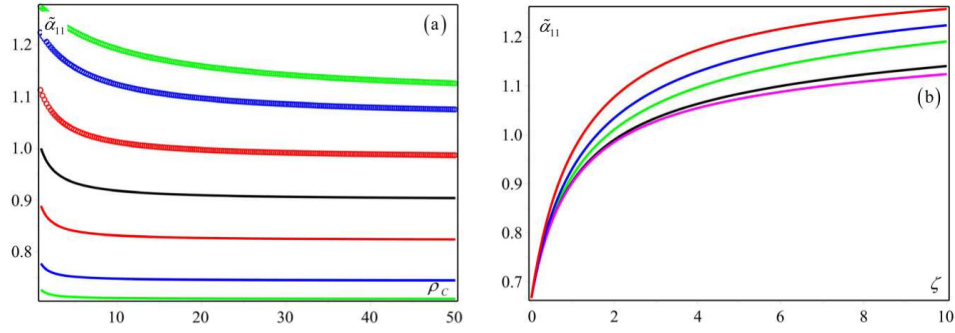


Figure 6: Dimensionless component $\tilde{\alpha}_{11}$ vs. the ratio ρ_C for $\tilde{\nu}_a = \tilde{\nu}_b = 0.3$, $\rho_\alpha = 2$ and for different values of the geometric ratio ζ : $\zeta = 1/10$ green line, $\zeta = 1/5$ blue line, $\zeta = 1/2$ red line, $\zeta = 1$ black line, $\zeta = 2$ red points, $\zeta = 5$ blue points, $\zeta = 10$ green points. (b) Dimensionless component α_{11} vs. the ratio ρ_C for $\tilde{\nu}_a = \tilde{\nu}_b = 0.3$, $\rho_\alpha = 2$ and for different values of the geometric ratio ρ_C : $\rho_C = 2$ red line, $\rho_C = 5$ blue line, $\rho_C = 10$ green line, $\rho_C = 30$ black line, $\rho_C = 50$ violet line.

$\tilde{K}_{iq_1} = 2/(1 + \rho_K)$. In the limit $\zeta \rightarrow +\infty$, for which the thickness of the layer b vanishes and $K_{iq_1} = K_{iq_1}^a$, the normalized components of the overall heat conductivity tensor tend to a finite value given by $\tilde{K}_{iq_1} = 2\rho_K/(1 + \rho_K)$. The non-dimensional components of the overall mass diffusion tensor \tilde{D}_{11} and \tilde{D}_{22} are characterized by properties similar to those of \tilde{K}_{11} and \tilde{K}_{22} , and can be studied substituting the non-dimensional ratio ρ_K with ρ_D .

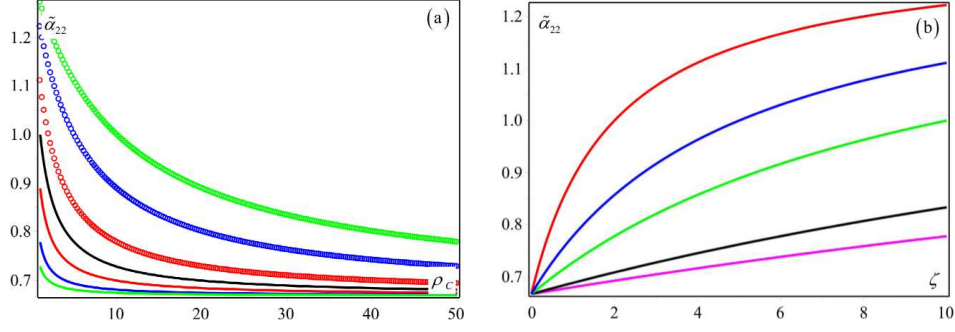


Figure 7: Dimensionless component $\tilde{\alpha}_{22}$ vs. the ratio ρ_C for $\tilde{\nu}_a = \tilde{\nu}_b = 0.3$, $\rho_\alpha = 2$ and for different values of the geometric ratio ζ : $\zeta = 1/10$ green line, $\zeta = 1/5$ blue line, $\zeta = 1/2$ red line, $\zeta = 1/1$ black line, $\zeta = 2$ red points, $\zeta = 5$ blue points, $\zeta = 10$ green points. (b) Dimensionless component α_{22} vs. the ratio ρ_C for $\tilde{\nu}_a = \tilde{\nu}_b = 0.3$, $\rho_\alpha = 2$ and for different values of the geometric ratio ρ_C : $\rho_C = 2$ red line, $\rho_C = 5$ blue line, $\rho_C = 10$ green line, $\rho_C = 30$ black line, $\rho_C = 50$ violet line.

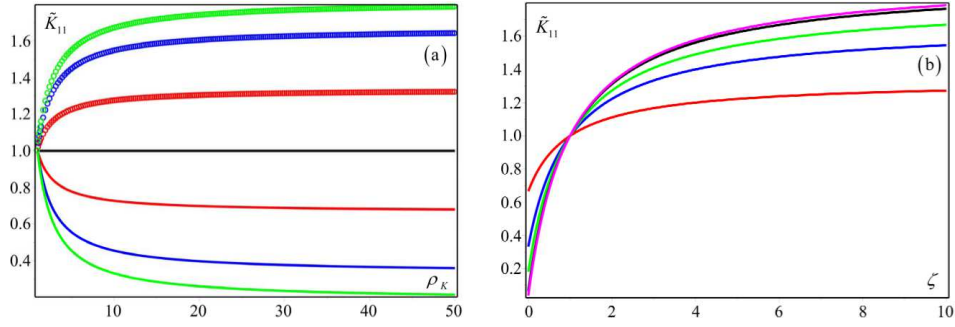


Figure 8: Dimensionless component \tilde{K}_{11} vs. the ratio ρ_K for different values of the geometric ratio ζ : $\zeta = 1/10$ green line, $\zeta = 1/5$ blue line, $\zeta = 1/2$ red line, $\zeta = 1/1$ black line, $\zeta = 2$ red points, $\zeta = 5$ blue points, $\zeta = 10$ green points. (b) Dimensionless component \tilde{K}_{11} vs. the ratio ρ_K for different values of the ratio ρ_K : $\rho_K = 2$ red line, $\rho_K = 5$ blue line, $\rho_K = 10$ green line, $\rho_K = 30$ black line, $\rho_K = 50$ violet line.

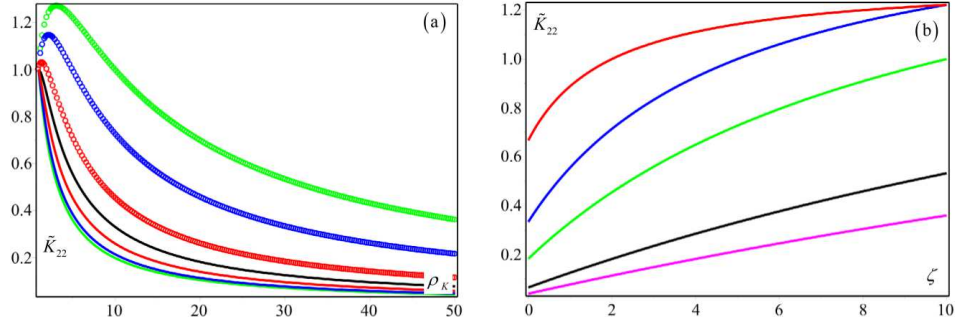


Figure 9: Dimensionless component \tilde{K}_{22} vs. the ratio ρ_K for different values of the geometric ratio ζ : $\zeta = 1/10$ green line, $\zeta = 1/5$ blue line, $\zeta = 1/2$ red line, $\zeta = 1/1$ black line, $\zeta = 2$ red points, $\zeta = 5$ blue points, $\zeta = 10$ green points. (b) Dimensionless component \tilde{K}_{22} vs. the ratio ρ_K for different values of the ratio ρ_K : $\rho_K = 2$ red line, $\rho_K = 5$ blue line, $\rho_K = 10$ green line, $\rho_K = 30$ black line, $\rho_K = 50$ violet line.

5.2 Comparative analysis: homogenized model vs heterogeneous material

In order to study the capabilities of the proposed homogenization procedure, the two-dimensional bi-phase orthotropic layered material shown in Fig. 2 is assumed to be subjected to \mathcal{L} -periodic harmonic body forces b_i , directed along the orthotropy direction x_j (see Fig. 2) and \mathcal{L} -periodic heat and mass sources $r(x_j)$ and $s(x_j)$:

$$b_j(x_j) = B_j e^{i \frac{2\pi m x_j}{L_j}}, \quad r(x_j) = R e^{i \frac{2\pi n x_j}{L_j}}, \quad s(x_j) = S e^{i \frac{2\pi p x_j}{L_j}}, \quad (40)$$

where: $j = 1, 2$; $L_1 = L_2 = L$; $B_i, R, S \in \mathbb{C}$; $m, n, p \in \mathbb{Z}$; and $i^2 = -1$.

This problem is analyzed by applying the homogenized first-order model with overall elastic and thermodiffusive constants derived from the homogenization of the periodic cell through the approach developed in previous Sections. The obtained results are then compared with those derived by means of a fully heterogeneous modelling procedure. Due to the periodicity of the heterogeneous material, body forces, heat and mass sources considered, only an horizontal (or vertical) characteristic portion of length L of the heterogeneous model is analyzed (Fig. 2b). In order to assess the reliability of the homogenized model, the macroscopic displacement, temperature and chemical potential fields are compared to the corresponding fields in the heterogeneous model by means of the up-scaling relations (17).

The overall elastic and thermodiffusive constants involving the fluctuation functions are obtained in exact analytical forms via expressions (33), (34), (35), (37), and (36). Conversely, the solution of the heterogeneous problem with \mathcal{L} -periodic harmonic body forces is computed via FE analysis with periodic boundary conditions on the displacement temperature and chemical potential fields. For the considered two-dimensional body subject to body forces along the orthotropy axes, heat and mass sources, the homogenized field equations (25)–(26) take the form:

$$C_{jjjj} \frac{\partial^2 U_j}{\partial x_j^2} - \alpha_{jj} \frac{\partial \Theta}{\partial x_j} - \beta_{jj} \frac{\partial \Upsilon}{\partial x_j} + b_j = 0, \quad K_{jj} \frac{\partial^2 \Theta}{\partial x_j^2} + r = 0, \quad D_{jj} \frac{\partial^2 \Upsilon}{\partial x_j^2} + s = 0, \quad (41)$$

where $j = 1, 2$ are not summed indexes. Equations (41) describe an extensional problem in presence of thermodiffusion. Considering body forces, heat and mass sources of the form (40), the macroscopic displacements, temperature and chemical potential fields are given by

$$U_j(x_j) = \frac{B_j L^2}{C_{jjjj} (2\pi m)^2} e^{i \frac{2\pi m x_j}{L_j}} - i \left[\frac{R \alpha_{jj} L^3}{C_{jjjj} K_{jj} (2\pi n)^3} e^{i \frac{2\pi n x_j}{L_j}} + \frac{S \beta_{jj} L^3}{C_{jjjj} D_{jj} (2\pi p)^3} e^{i \frac{2\pi p x_j}{L_j}} \right], \quad (42)$$

$$\Theta(x_j) = \frac{R L^2}{K_{jj} (2\pi n)^2} e^{i \frac{2\pi n x_j}{L_j}}, \quad \Upsilon(x_j) = \frac{S L^2}{D_{jj} (2\pi p)^2} e^{i \frac{2\pi p x_j}{L_j}}, \quad (43)$$

where $j = 1, 2$ are still not summed indexes. In order to compare the behavior of the derived analytical solution with the numerical results provided by the heterogeneous model, only the real part of macroscopic fields (42), (43) is accounted. Moreover, the imaginary part of the amplitudes B_j , R and S is assumed to be zero. The real part of expressions (42), (43) can be written in the non-dimensional form:

$$U_j^*(x_j) = \cos\left(\frac{2\pi m x_j}{L_j}\right) + \Xi_{jj}^\alpha \frac{m^2}{2\pi n^3} \sin\left(\frac{2\pi n x_j}{L_j}\right) + \Xi_{jj}^\beta \frac{m^2}{2\pi p^3} \sin\left(\frac{2\pi p x_j}{L_j}\right), \quad (44)$$

$$\Theta^*(x_j) = \cos\left(\frac{2\pi n x_j}{L_j}\right), \quad \Upsilon^*(x_j) = \cos\left(\frac{2\pi p x_j}{L_j}\right), \quad (45)$$

where $U_j^* = \frac{U_j C_{jjjj}(2\pi m)^2}{B_j L_j^2}$, $\Theta^* = \frac{\Theta K_{jj}(2\pi n)^2}{R L_j^2}$, $\Upsilon^* = \frac{\Upsilon D_{jj}(2\pi p)^2}{S L_j^2}$; and $\Xi_{jj}^\alpha = \frac{\alpha_{jj} R L_j}{K_{jj} B_j}$ and $\Xi_{jj}^\beta = \frac{\beta_{jj} S L_j}{D_{jj} B_j}$, $j = 1, 2$ are still not summed indexes.

The amplitude functions Ξ_{jj}^α and Ξ_{jj}^β are associated respectively with the thermal expansion and mass diffusion contribution to the macroscopic displacement (44) along the direction \mathbf{e}_j . In order to study the influence of the geometrical, elastic and thermodiffusive properties of the phases on Ξ_{jj}^α and Ξ_{jj}^β , the following non-dimensional form for these functions is introduced:

$$\tilde{\Xi}_{jj}^\alpha(\rho_C, \rho_\alpha, \rho_K, \zeta, \tilde{\nu}_a, \tilde{\nu}_b) = \frac{\Xi_{jj}^\alpha}{\hat{\Xi}_{jj}^\alpha}, \quad \tilde{\Xi}_{jj}^\beta(\rho_C, \rho_\beta, \rho_K, \zeta, \tilde{\nu}_a, \tilde{\nu}_b) = \frac{\Xi_{jj}^\beta}{\hat{\Xi}_{jj}^\beta}, \quad \text{with } j = 1, 2, \quad (46)$$

where $\hat{\Xi}_{jj}^\alpha = R L_j (\alpha^a + \alpha^b) / B_j (K^a + K^b)$ and $\hat{\Xi}_{jj}^\beta = R L_j (\beta^a + \beta^b) / B_j (D^a + D^b)$. In the case where the two phases possess the same value of the Poisson's coefficient ($\tilde{\nu}_a = \tilde{\nu}_b$), the following property is verified for the normalized amplitude functions:

$$\tilde{\Xi}_{jj}^\alpha(\rho_C, \rho_\alpha, \rho_K, \zeta, \tilde{\nu}) = \tilde{\Xi}_{jj}^\alpha(\rho_C^{-1}, \rho_\alpha^{-1}, \rho_K^{-1}, \tilde{\nu}), \quad \tilde{\Xi}_{jj}^\beta(\rho_C, \rho_\beta, \rho_K, \zeta, \tilde{\nu}) = \tilde{\Xi}_{jj}^\beta(\rho_C^{-1}, \rho_\alpha^{-1}, \rho_K^{-1}, \tilde{\nu}). \quad (47)$$

The three-dimensional plot reported in Fig. 10/(a) shows the variation of the normalized amplitude component $\tilde{\Xi}_{11}^\alpha$ with ρ_α and ρ_K for $\tilde{\nu}_a = \tilde{\nu}_b = 0.3$, $\rho_C = 10$ and $\zeta = 1$. In Fig. 10/(b) the same component $\tilde{\Xi}_{11}^\alpha$, which represents the contribution of the thermal expansion to the macroscopic displacement along the direction \mathbf{e}_1 , is plotted as a function of ρ_C assuming $\tilde{\nu}_a = \tilde{\nu}_b = 0.3$, $\rho_\alpha = \rho_K = 10$ and several values of the dimensionless ratio ζ . The variation of the normalized component $\tilde{\Xi}_{22}^\alpha$, corresponding to the contribution of the thermal expansion to the macroscopic displacement along \mathbf{e}_2 (see Fig. 2), is reported in Fig. 11/(a) as a function of ρ_α and ρ_K for $\tilde{\nu}_a = \tilde{\nu}_b = 0.3$, $\rho_C = 10$ and $\zeta = 1$, and in Fig. 11/(b) as a function of ρ_C assuming $\tilde{\nu}_a = \tilde{\nu}_b = 0.3$, $\rho_\alpha = \rho_K = 10$. Observing the curves reported in the figures, it can be noted that the normalized amplitude $\tilde{\Xi}_{22}^\alpha$, associate to the component of the macroscopic displacement $U_2^*(x_2)$ parallel to the stratification direction, is greater than the amplitude $\tilde{\Xi}_{11}^\alpha$ which correspond to the component $U_1^*(x_1)$ parallel to the stratification direction. The dimensionless amplitude $\tilde{\Xi}_{11}^\beta$ and $\tilde{\Xi}_{22}^\beta$, associated to the contributions of the mass diffusion respectively to $U_1^*(x_1)$ and $U_2^*(x_2)$, are characterized by the same properties of $\tilde{\Xi}_{11}^\alpha$ and $\tilde{\Xi}_{22}^\alpha$, and their behavior can be easily studied substituting the non-dimensional ratios ρ_α and ρ_K with ρ_β and ρ_D .

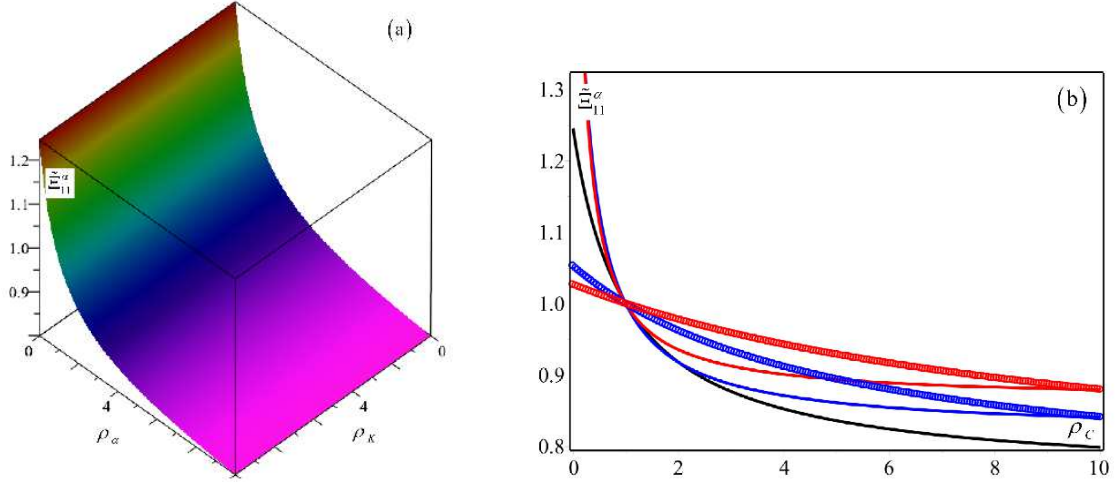


Figure 10: (a) Dimensionless amplitude $\tilde{\Xi}_{11}^\alpha$ vs. the ratios ρ_α and ρ_K for $\tilde{\nu}_a = \tilde{\nu}_b = 0.3$, $\rho_C=10$ and $\zeta = 1$. (b) Dimensionless amplitude $\tilde{\Xi}_{11}^\alpha$ vs. the ratios ρ_C for $\tilde{\nu}_a = \tilde{\nu}_b = 0.3$, $\rho_\alpha = \rho_K = 10$ and $\zeta = 1$ for different values of the geometric ratio ζ : $\zeta = 1/10$ red line, $\zeta = 1/5$ blue line, $\zeta = 1$ black line, $\zeta = 5$ blue line points, $\zeta = 10$ red line points.

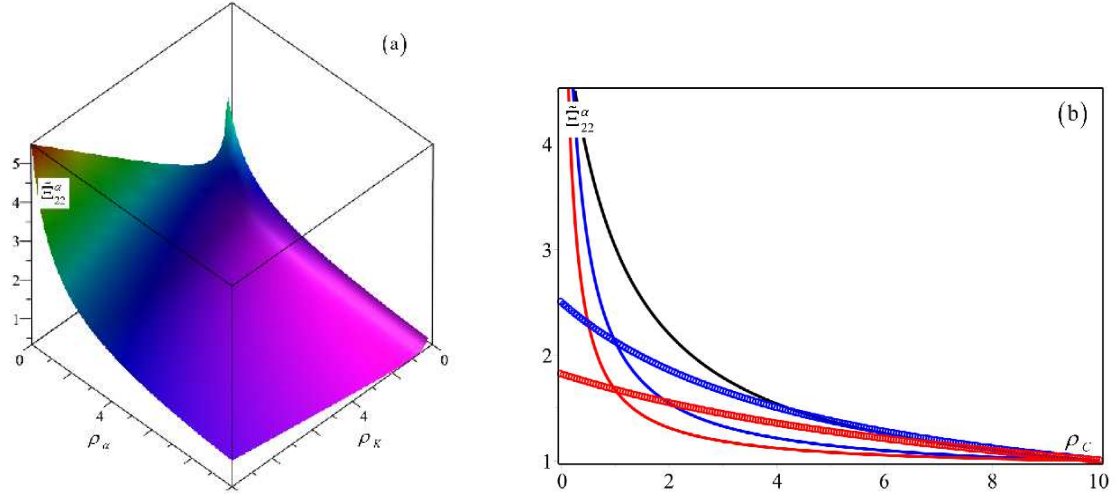


Figure 11: (a) Dimensionless amplitude $\tilde{\Xi}_{22}^\alpha$ vs. the ratios ρ_α and ρ_K for $\tilde{\nu}_a = \tilde{\nu}_b = 0.3$, $\rho_C=10$ and $\zeta = 1$. (b) Dimensionless amplitude $\tilde{\Xi}_{22}^\alpha$ vs. the ratios ρ_C for $\tilde{\nu}_a = \tilde{\nu}_b = 0.3$, $\rho_\alpha = \rho_K = 10$ and $\zeta = 1$ for different values of the geometric ratio ζ : $\zeta = 1/10$ red line, $\zeta = 1/5$ blue line, $\zeta = 1$ black line, $\zeta = 5$ blue line points, $\zeta = 10$ red line points.

The analytical solution (44) and (45), derived by the solution of the homogenized field equations (41) is now compared with the results obtained by the finite element analysis of the heterogeneous problem corresponding to the bi-phase layered material reported in Fig. 2 subject to harmonic body forces, heat and mass sources. More precisely, finite element analysis of the heterogeneous problem, performed by means of the program COMSOL Multiphysics, provides the local fields u_j , θ , η which are used together with the *up-scaling* relations (17) for obtaining the macroscopic fields U_j , Θ and Υ . These macroscopic quantities are compared with the analytical expressions (44) and (45). Plane stress condition has been assumed for both the solution of the homogenized equations and the heterogeneous problem, and two isotropic phases with the same value of the Poisson's coefficient $\nu_a = \nu_b = 0.3$ have been considered.

In Fig. 12, the macroscopic displacement component U_1^* and temperature Θ^* evaluated using analytical expressions (44) and (45)₁ are reported as functions of the normalized spatial coordinate x_1/L (continuous lines in the figure) and compared with the numerical results obtained by the heterogeneous model assuming periodic body forces $b_1(x_1)$ and heat sources $r(x_1)$ and considering the value of the amplitude $\Xi_{11}^\alpha = 1$ (diamonds in the figure). The following values for the geometrical parameters, the ratios between the elastic and of thermodiffusive constants have been assumed: $L/\varepsilon = 10$, $\rho_C = 10$, $\rho_\alpha = 10$, $\rho_\beta = 0$, $\rho_K = 10$, $\rho_D = 0$, the effects of the mass diffusion have been neglected in this example. The macroscopic displacement and temperature fields are plotted for the characteristic portion of length $L_1 = L$, corresponding to $x_1/L = 1$ (i. e. for $0 \leq x_1/L \leq 1$), and several values for the wave numbers $m, n \in \mathbb{Z}$ have been considered. Observing the curves, for both the quantities $U_1^*(x_1/L)$ and $\Theta^*(x_1/L)$ a good agreement is detected between the results derived by means of the first order homogenization approach and those obtained by the heterogeneous model.

Results for the macroscopic displacement component U_2^* and temperature in Θ^* along the characteristic portion of length $L_2 = L$ in direction parallel to \mathbf{e}_2 (not reported here for conciseness) show a good agreement between the solution obtained by means of the first-order asymptotic homogenization method and the values obtained by means of finite element analysis of the heterogeneous problem.

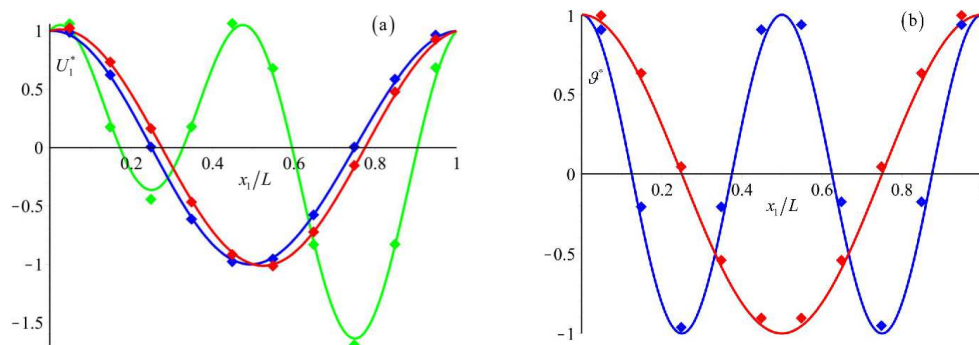


Figure 12: Macroscopic displacement component U_1^* and temperature fields Θ^* due to harmonic body force b_1 and temperature source r . The heterogeneous model (diamonds) is compared with the homogenized first order model. (a) Dimensionless macro displacement U_1^* vs. the ratio x_1/L for $\Xi_{11}^\alpha = 1$ for different values of wave number n, m ($n = 1, m = 1$ red line; $n = 2, m = 1$ blue line; $n = 1, m = 2$ green line). (b) Macro temperature Θ^* vs. the ratio x_1/L for different values of wave number n ($n = 1$ red line; $n = 2$, blue line).

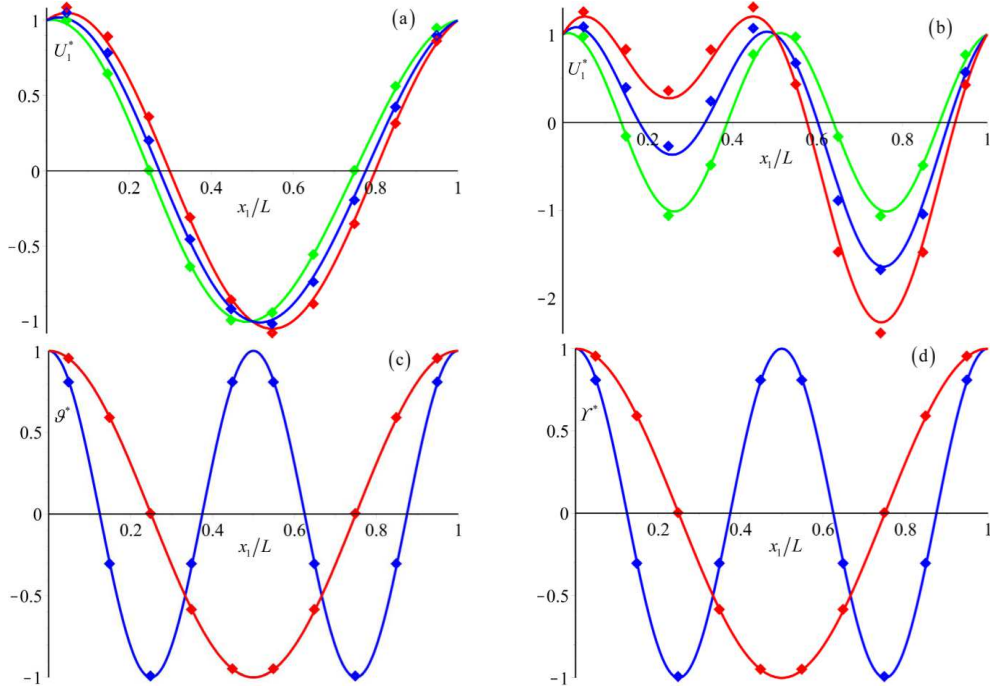


Figure 13: Macroscopic displacement component U_1^* , temperature Θ^* , and chemical potential Υ^* due to harmonic body force b_1 and temperature and mass sources r, s respectively. The heterogeneous model (diamonds) is compared with the homogenized first order model. Dimensionless macro displacement U_1^* vs. the ratio x_1/L for $\Xi_{11}^\alpha = 1, \Xi_{11}^\beta = 1$ and wave number $m = 1$ (a), $m = 2$ (b) for different values of wave number n , p ($n = 1$, $p = 1$ red line; $n = 2$, $p = 1$ blue line; $n = 2$, $p = 2$ green line). (c) Macro temperature Θ^* vs. the ratio x_1/L for different values of wave number n ($n = 1$ red line; $n = 2$, blue line). (d) Macro concentration Υ^* vs. the ratio x_1/L for different values of wave number p ($p = 1$ red line; $p = 2$, blue line).

In Fig. 13, the variation of the normalized component of the macroscopic displacement $U_1^*(x_1/L)$, temperature $\Theta^*(x_1/L)$ and chemical potential $\Upsilon^*(x_1/L)$ along the characteristic portion of length $L_1 = L$ is plotted as a function of x_1/L . Two isotropic phases having the same Poisson's coefficient $\nu = 0.3$ have been assumed, and the same values of the previous example have been assigned to the geometrical, elastic and thermal parameters. The amplitude of the mass diffusion contribution to the displacement is assumed to be $\tilde{\Xi}_{11}^\beta = 1$, and $\rho_K = 10$. Similarly to the previous case, for the finite element analysis of the heterogeneous elastic thermodiffusive problem harmonic body forces $b_1(x_1)$, heat and mass sources $r(x_1)$ and $s(x_1)$ have been introduced. The reported curves show a good agreement between the results obtained by the asymptotic homogenization (continuous lines the figure) and those provided by the heterogeneous elastic thermodiffusive model (diamonds in the figure). The good agreement between the results coming from the two different approaches can be observed for $U_1^*(x_1/L)$ in Fig. 13/(a), (b), for $\Theta^*(x_1/L)$ in Fig. 13/(c) and for $\Upsilon^*(x_1/L)$ in Fig. 13/(d). Similar results are obtained for the macroscopic displacement U_2^* , temperature Θ^* and chemical potential Υ^* along the characteristic portion of length $L_2 = L$ in direction parallel to \mathbf{e}_2 .

6 Conclusions

A general asymptotic homogenization approach for describing the static elastic, thermal and diffusive properties of periodic composite materials in presence of thermodiffusion is proposed. *Down-scaling* relations associating the displacements, temperature and chemical potential at the micro-scale to the corresponding fields at the macro-scale are introduced. Perturbation functions are defined for representing the effects of the microstructures on the microscopic displacement, temperature, chemical potential and on the coupling effects between these fields. These perturbation functions are obtained through the solution of non-homogeneous problems on the cell defining periodic boundary conditions and normalization conditions (*up-scaling* relations).

Averaged field equations of infinite order are derived for the considered class of periodic thermodiffusive materials, and an original formal solution is performed by means of power series expansion of the macroscopic displacements, temperature and chemical potential fields. Field equation for the homogenized Cauchy thermodiffusive continuum are derived, and exact expressions for the overall elastic and thermodiffusive constants of this equivalent first order medium are obtained.

An example of application of the developed general method to the illustrative case of a two-dimensional bi-phase orthotropic layered material is provided. The effective elastic and thermodiffusive constants of this particular composite material are determined using the general expressions derived by the asymptotic homogenization procedure. Analytical expressions for the macroscopic fields derived by the solution of the homogenized equations corresponding to the first order equivalent continuum. Finite element analysis of the corresponding heterogeneous model is performed assuming periodic body forces, heat and mass sources acting on the considered bi-phase layered composite. In order to compare the analytical solution of the homogenized equations with the numerical results obtained by the heterogeneous model, the microscopic fields computed by finite elements techniques are used to estimate the macroscopic displacements, temperature and chemical potential fields by means of the *up-scaling* relations defined in the paper. The good agreement detected between the solution derived by the homogenized first order equations and the numerical results obtained by the heterogeneous model through the *up-scaling* relations represents an important validation of the accuracy of the proposed asymptotic homogenization approach.

Thanks to the great versatility of the asymptotic homogenization techniques and to the proposed general rigorous formulation, the method developed in the paper can be adopted for studying effective elastic and thermodiffusive properties of many composite materials, without any other assumption regarding the geometry of the microstructures in addition to the periodicity. In particular, the proposed asymptotic homogenization procedure can have relevant applications in modelling mechanical and thermodiffusive properties of energy devices with layered configurations, such as lithium ions batteries and solid oxide fuel cells. In standard operative situations, the components of these devices are commonly subject to severe thermomechanical and diffusive stress which can cause damages and crack formation compromising their performances. Consequently, evaluating the overall elastic and thermodiffusive properties of these battery devices through the asymptotic homogenization approach illustrated in the paper can represent an important issue in order to predict damaging phenomena and to improve the efficient design and manufacturing of these systems.

Multi-scale homogenization techniques such as that proposed in the paper provide an accurate description of the macroscopical mechanical and thermodiffusive properties of heterogeneous materials through the derivation of effective constants of the first order equivalent continuum. Nevertheless, first order homogenization procedures are not enough accurate to model size-effects and non-local phenomena connected to the microstructural scale length. As a consequence, the devel-

oped first order homogenization approach does not provide a precise description of the behavior of thermodiffusive composite materials in presence of high gradients of stresses, deformations, temperature, chemical potential, heat and mass fluxes, as well as of non-local phenomena such as waves dispersion. In order to overcome these limits in the accuracy, non-local higher order homogenization techniques can be used. These methods provide constitutive relations of equivalent higher order continuum media including characteristic scale-lengths associate to the microstructural effects. Using the rigorous and general approach illustrated in the paper, a better approximation of the elastic and thermodiffusive behavior of composite materials in presence of strong gradients can be obtained through the solution of higher order cells problems involving the coefficients of the averaged field equations of infinite order reported in Appendix A. As it is shown in the same Appendix, these equations can be formally solved by means of a double asymptotic expansion performed in terms of the microstructural size.

Acknowledgments

AB and LM gratefully acknowledge financial support from the Italian Ministry of Education, University and Research in the framework of the FIRB project 2010 "Structural mechanics models for renewable energy applications". AP would like to acknowledge financial support from the European Union's Seventh Framework Programme FP7/2007-2013/ under REA Grant agreement number PCIG13-GA-2013-618375-MeMic.

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A Higher-order analysis and averaged equations of infinite order

In this Appendix, explicit expressions for the higher order cells problems associated to the *down-scaling* relations (12), (13) and (14) are reported. Moreover, the averaged field equations of infinite order are derived, and a formal solution is obtained by means of an asymptotic expansion of the macroscopic fields in terms of the microstructural size.

A.1 Higher-order asymptotic analysis and derivation of the corresponding cell problems

In order to derive exact expressions for the fluctuation functions affecting the behavior of the microscopic fields u_k, θ, η , the *down-scaling* relations (12), (13) and (14) are substituted into the microscopic field equations (7), (8). Remembering the property $\frac{\partial}{\partial x_j} f(\mathbf{x}, \boldsymbol{\xi} = \frac{\mathbf{x}}{\varepsilon}) = \left(\frac{\partial f}{\partial x_j} + \frac{1}{\varepsilon} \frac{\partial f}{\partial \xi_j} \right)_{\boldsymbol{\xi}=\mathbf{x}/\varepsilon} = \left(\frac{\partial f}{\partial x_j} + \frac{f_{,j}}{\varepsilon} \right)_{\boldsymbol{\xi}=\mathbf{x}/\varepsilon}$, equation (7) become

$$\begin{aligned}
& \varepsilon^{-1} \left\{ \left[\left(C_{ijkl}^\varepsilon N_{kpq_1, l}^{(1)} \right)_{,j} + C_{ijpq_1, j}^\varepsilon \right] H_{pq_1}(\mathbf{x}) + \left[\left(C_{ijkl}^\varepsilon \tilde{N}_{k, l}^{(1)} \right)_{,j} - \alpha_{ij, j}^\varepsilon \right] \Theta(\mathbf{x}) \right. \\
& \quad \left. + \left[\left(C_{ijkl}^\varepsilon \hat{N}_{k, l}^{(1)} \right)_{,j} - \beta_{ij, j}^\varepsilon \right] \Upsilon(\mathbf{x}) \right\} \\
& + \varepsilon^0 \left\{ \left(C_{ijkl}^\varepsilon N_{kpq_1 q_2, l}^{(2)} \right)_{,j} + \frac{1}{2} \left(\left(C_{ijkq_2}^\varepsilon N_{kpq_1}^{(1)} \right)_{,j} + C_{iq_2 pq_1}^\varepsilon + C_{iq_2 kl}^\varepsilon N_{kpq_1, l}^{(1)} \right. \right. \\
& \quad \left. \left. + \left(C_{ijkq_1}^\varepsilon N_{kpq_2}^{(1)} \right)_{,j} + C_{iq_1 pq_2}^\varepsilon + C_{iq_1 kl}^\varepsilon N_{kpq_2, l}^{(1)} \right) \kappa_{pq_1 q_2}(\mathbf{x}) \right. \\
& \quad \left. + \left[\left(C_{ijkl}^\varepsilon \tilde{N}_{kq_1, l}^{(2)} \right)_{,j} + \left(C_{ijkq_1}^\varepsilon \tilde{N}_k^{(1)} \right)_{,j} + C_{iq_1 kl}^\varepsilon \tilde{N}_{k, l}^{(1)} - \alpha_{iq_1}^\varepsilon - \left(\alpha_{ij}^\varepsilon M_{q_1}^{(1)} \right)_{,j} \right] \frac{\partial \Theta}{\partial x_{q_1}} \right. \\
& \quad \left. + \left[\left(C_{ijkl}^\varepsilon \hat{N}_{kq_1, l}^{(2)} \right)_{,j} + \left(C_{ijkq_1}^\varepsilon \hat{N}_k^{(1)} \right)_{,j} + C_{iq_1 kl}^\varepsilon \hat{N}_{k, l}^{(1)} - \beta_{iq_1}^\varepsilon - \left(\beta_{ij}^\varepsilon W_{q_1}^{(1)} \right)_{,j} \right] \frac{\partial \Upsilon}{\partial x_{q_1}} \right\} \\
& + \dots + b_i(\mathbf{x}) = 0, \quad i = 1, 2,
\end{aligned} \tag{48}$$

where $H_{pq_1} = \partial U_p / \partial x_{q_1}$ are the components of the macroscopic displacement gradient tensor previously defined, and $\kappa_{pq_1 q_2} = \partial^2 U_p / \partial x_{q_1} \partial x_{q_2}$ are the elements of the macroscopic second gradient tensor. Equations (8) assume the following form

$$\begin{aligned} & \varepsilon^{-1} \left[\left(K_{ij}^\varepsilon M_{q_1, j}^{(1)} \right)_{,i} + K_{iq_1, i}^\varepsilon \right] \frac{\partial \Theta}{\partial x_{q_1}} \\ & + \varepsilon^0 \left[\left(K_{ij}^\varepsilon M_{q_1 q_2, j}^{(2)} \right)_{,i} + \frac{1}{2} \left(\left(K_{iq_1}^\varepsilon M_{q_2}^{(1)} \right)_{,i} + K_{q_2 q_1}^\varepsilon + K_{q_1 j}^\varepsilon M_{q_2, j}^{(1)} \right. \right. \\ & \quad \left. \left. + \left(K_{iq_2}^\varepsilon M_{q_1}^{(1)} \right)_{,i} + K_{q_1 q_2}^\varepsilon + K_{q_2 j}^\varepsilon M_{q_1, j}^{(1)} \right) \right] \frac{\partial^2 \Theta}{\partial x_{q_1} \partial x_{q_2}} \\ & + \dots + r(\mathbf{x}) = 0, \end{aligned} \quad (49)$$

$$\begin{aligned} & \varepsilon^{-1} \left[\left(D_{ik}^\varepsilon W_{q_1, j}^{(1)} \right)_{,i} + D_{iq_1, i}^\varepsilon \right] \frac{\partial \Upsilon}{\partial x_{q_1}} \\ & + \varepsilon^0 \left[\left(D_{ij}^\varepsilon W_{q_1 q_2, j}^{(2)} \right)_{,i} + \frac{1}{2} \left(\left(D_{iq_1}^\varepsilon W_{q_2}^{(1)} \right)_{,i} + D_{q_2 q_1}^\varepsilon + D_{q_1 j}^\varepsilon W_{q_2, j}^{(1)} \right. \right. \\ & \quad \left. \left. + \left(D_{iq_2}^\varepsilon W_{q_1}^{(1)} \right)_{,i} + D_{q_1 q_2}^\varepsilon + D_{q_2 j}^\varepsilon W_{q_1, j}^{(1)} \right) \right] \frac{\partial^2 \Upsilon}{\partial x_{q_1} \partial x_{q_2}} \\ & + \dots + s(\mathbf{x}) = 0. \end{aligned} \quad (50)$$

In order to transform the field equations (48), (49) and (50) in a PDEs system with constant coefficients, in which the unknowns are the macroscopic quantities $U_k(\mathbf{x})$, $\Theta(\mathbf{x})$ and $\Upsilon(\mathbf{x})$, the fluctuation functions have to satisfy non-homogeneous equations (*cell problems*) reported below.

At the order ε^{-1} from the equations (48), (49), (50) we derive the *first-order cell problems* reported in Sec. 3.2 in the text of the paper, equations (21) and (22).

At the order ε^0 , equation (48) yields the following *second-order cell problems*

$$\begin{aligned} & \left(C_{ijkl}^\varepsilon N_{kpq_1 q_2, l}^{(2)} \right)_{,j} + \frac{1}{2} \left[\left(C_{ijkq_2}^\varepsilon N_{kpq_1}^{(1)} \right)_{,j} + C_{iq_2 pq_1}^\varepsilon + C_{iq_2 kl}^\varepsilon N_{kpq_1, l}^{(1)} \right. \\ & \quad \left. + \left(C_{ijkq_1}^\varepsilon N_{kpq_2}^{(1)} \right)_{,j} + C_{iq_1 pq_2}^\varepsilon + C_{iq_1 kl}^\varepsilon N_{kpq_2, l}^{(1)} \right] = n_{ipq_1 q_2}^{(2)}, \\ & \left(C_{ijkl}^\varepsilon \tilde{N}_{kq_1, l}^{(2)} \right)_{,j} + \left(C_{ijkq_1}^\varepsilon \tilde{N}_k^{(1)} \right)_{,j} + C_{iq_1 kl}^\varepsilon \tilde{N}_{k, l}^{(1)} - \alpha_{iq_1}^\varepsilon - \left(\alpha_{ij}^\varepsilon M_{q_1}^{(1)} \right)_{,j} = \tilde{n}_{iq_1}^{(2)}, \\ & \left(C_{ijkl}^\varepsilon \hat{N}_{kq_1, l}^{(2)} \right)_{,j} + \left(C_{ijkq_1}^\varepsilon \hat{N}_k^{(1)} \right)_{,j} + C_{iq_1 kl}^\varepsilon \hat{N}_{k, l}^{(1)} - \beta_{iq_1}^\varepsilon - \left(\beta_{ij}^\varepsilon W_{q_1}^{(1)} \right)_{,j} = \hat{n}_{iq_1}^{(2)} \end{aligned} \quad (51)$$

At the same order, from (49), (50) we derive the *second-order thermodiffusive cell problems*:

$$\begin{aligned} & \left(K_{ij}^\varepsilon M_{q_1 q_2, j}^{(2)} \right)_{,i} + \frac{1}{2} \left[\left(K_{iq_1}^\varepsilon M_{q_2}^{(1)} \right)_{,i} + K_{q_2 q_1}^\varepsilon + K_{q_1 j}^\varepsilon M_{q_2, j}^{(1)} \right. \\ & \quad \left. + \left(K_{iq_2}^\varepsilon M_{q_1}^{(1)} \right)_{,i} + K_{q_1 q_2}^\varepsilon + K_{q_2 j}^\varepsilon M_{q_1, j}^{(1)} \right] = m_{q_1 q_2}^{(2)}, \end{aligned} \quad (52)$$

$$\begin{aligned} & \left(D_{ij}^\varepsilon W_{q_1 q_2, j}^{(2)} \right)_{,i} + \frac{1}{2} \left[\left(D_{i q_1}^\varepsilon W_{q_2}^{(1)} \right)_{,i} + D_{q_2 q_1}^\varepsilon + D_{q_1 j}^\varepsilon W_{q_2, j}^{(1)} \right. \\ & \left. + \left(D_{i q_2}^\varepsilon W_{q_1}^{(1)} \right)_{,i} + D_{q_1 q_2}^\varepsilon + D_{q_2 j}^\varepsilon W_{q_1, j}^{(1)} \right] = w_{q_1 q_2}^{(2)}, \end{aligned} \quad (53)$$

where:

$$\begin{aligned} n_{ipq_1 q_2}^{(2)} &= \frac{1}{2} \left\langle C_{i q_2 p q_1}^\varepsilon + C_{i q_2 k l}^\varepsilon N_{k p q_1, l}^{(1)} + C_{i q_1 p q_2}^\varepsilon + C_{i q_1 k l}^\varepsilon N_{k p q_2, l}^{(1)} \right\rangle, \\ \tilde{n}_{i q_1}^{(2)} &= \left\langle C_{i q_1 k l}^\varepsilon \tilde{N}_{k, l}^{(1)} - \alpha_{i q_1}^\varepsilon \right\rangle, \quad \hat{n}_{i q_1}^{(2)} = \left\langle C_{i q_1 k l}^\varepsilon \hat{N}_{k, l}^{(1)} - \beta_{i q_1}^\varepsilon \right\rangle, \\ m_{q_1 q_2}^{(2)} &= \frac{1}{2} \left\langle K_{q_2 q_1}^\varepsilon + K_{q_1 j}^\varepsilon M_{q_2, j}^{(1)} + K_{q_1 q_2}^\varepsilon + K_{q_2 j}^\varepsilon M_{q_1, j}^{(1)} \right\rangle, \\ w_{q_1 q_2}^{(2)} &= \frac{1}{2} \left\langle D_{q_2 q_1}^\varepsilon + D_{q_1 j}^\varepsilon W_{q_2, j}^{(1)} + D_{q_1 q_2}^\varepsilon + D_{q_2 j}^\varepsilon W_{q_1, j}^{(1)} \right\rangle. \end{aligned} \quad (54)$$

In general, for the $m = 1, 2, \dots$, the m -order *cell problems* associate to equation (48) assume the form:

$$\begin{aligned} & \left(C_{ij kl}^\varepsilon N_{k p q_1 \dots q_m, l}^{(m)} \right)_{,j} + \frac{1}{m!} \sum_{\mathcal{P}(q)} \left[\left(C_{ij k q_m}^\varepsilon N_{k p q_1 \dots q_{m-1}}^{(m-1)} \right)_{,j} + C_{i q_m k q_{m-1}}^\varepsilon N_{k p q_1 \dots q_{m-2}}^{(m-2)} \right. \\ & \left. + C_{i q_m k l}^\varepsilon N_{k p q_1 \dots q_{m-1}, l}^{(m-1)} \right] = n_{ipq_1 \dots q_m}^{(m)}, \\ & \left(C_{ij kl}^\varepsilon \tilde{N}_{k q_1 \dots q_{m-1}, l}^{(m)} \right)_{,j} + \frac{1}{m!} \sum_{\mathcal{P}(q)} \left[\left(C_{ij k q_{m-1}}^\varepsilon \tilde{N}_{k q_1 \dots q_{m-2}}^{(m-1)} \right)_{,j} + C_{i q_{m-1} k q_{m-2}}^\varepsilon \tilde{N}_{k q_1 \dots q_{m-3}}^{(m-2)} \right. \\ & \left. + C_{i q_{m-1} k l}^\varepsilon \tilde{N}_{q_1 \dots q_{m-2}, l}^{(m-1)} - \alpha_{i q_{m-1}}^\varepsilon M_{q_1 \dots q_{m-2}}^{(m-2)} - \left(\alpha_{ij}^\varepsilon M_{q_1 \dots q_{m-1}}^{(m-1)} \right)_{,j} \right] = \tilde{n}_{i q_1 \dots q_{m-1}}^{(m)}, \\ & \left(C_{ij kl}^\varepsilon \hat{N}_{k q_1 \dots q_{m-1}, l}^{(m)} \right)_{,j} + \frac{1}{m!} \sum_{\mathcal{P}(q)} \left[\left(C_{ij k q_{m-1}}^\varepsilon \hat{N}_{k q_1 \dots q_{m-2}}^{(m-1)} \right)_{,j} + C_{i q_{m-1} k q_{m-2}}^\varepsilon \hat{N}_{k q_1 \dots q_{m-3}}^{(m-2)} \right. \\ & \left. + C_{i q_{m-1} k l}^\varepsilon \hat{N}_{q_1 \dots q_{m-2}, l}^{(m-1)} - \beta_{i q_{m-1}}^\varepsilon W_{q_1 \dots q_{m-2}}^{(m-2)} - \left(\beta_{ij}^\varepsilon W_{q_1 \dots q_{m-1}}^{(m-1)} \right)_{,j} \right] = \hat{n}_{i q_1 \dots q_{m-1}}^{(m)}, \end{aligned} \quad (55)$$

whereas the m -order thermodiffusive *cell problems* corresponding to equations (49) and (50) are:

$$\begin{aligned} & \left(K_{ij}^\varepsilon M_{q_1 \dots q_m, j}^{(m)} \right)_{,i} + \frac{1}{m!} \sum_{\mathcal{P}(q)} \left[\left(K_{i q_m}^\varepsilon M_{q_1 \dots q_{m-1}}^{(m-1)} \right)_{,i} \right. \\ & \left. + K_{q_m q_1}^\varepsilon M_{q_2 \dots q_{m-1}}^{(m-2)} + K_{q_m j}^\varepsilon M_{q_1 \dots q_{m-1}, j}^{(m-1)} \right] = m_{q_1 \dots q_m}^{(m)}, \end{aligned} \quad (56)$$

$$\begin{aligned} & \left(D_{ij}^\varepsilon W_{q_1 \dots q_m, j}^{(m)} \right)_{,i} + \frac{1}{m!} \sum_{\mathcal{P}(q)} \left[\left(D_{i q_m}^\varepsilon W_{q_1 \dots q_{m-1}}^{(m-1)} \right)_{,i} \right. \\ & \left. + D_{q_m q_1}^\varepsilon W_{q_2 \dots q_{m-1}}^{(m-2)} + D_{q_m j}^\varepsilon W_{q_1 \dots q_{m-1}, j}^{(m-1)} \right] = w_{q_1 \dots q_m}^{(m)}, \end{aligned} \quad (57)$$

where the symbol $\mathcal{P}(q)$ denotes all possible permutations of the multi-index q , and the constants $n_{ipq_1 \dots q_m}^{(m)}$, $\tilde{n}_{iq_1 \dots q_{m-1}}^{(m)}$, $\hat{n}_{iq_1 \dots q_{m-1}}^{(m)}$, $m_{q_1 \dots q_m}^{(m)}$, $w_{q_1 \dots q_m}^{(m)}$ are defined as follows:

$$\begin{aligned}
n_{ipq_1 \dots q_m}^{(m)} &= \frac{1}{m!} \sum_{\mathcal{P}(q)} \left\langle C_{iq_m k q_{m-1}}^\varepsilon N_{kpq_1 \dots q_{m-2}}^{(m-2)} + C_{iq_m kl}^\varepsilon N_{kpq_1 \dots q_{m-1}, l}^{(m-1)} \right\rangle, \\
\tilde{n}_{iq_1 \dots q_{m-1}}^{(m)} &= \frac{1}{m!} \sum_{\mathcal{P}(q)} \left\langle C_{iq_{m-1} k q_{m-2}}^\varepsilon \tilde{N}_{kq_1 \dots q_{m-3}}^{(m-2)} + C_{iq_{m-1} kl}^\varepsilon \tilde{N}_{q_1 \dots q_{m-2}, l}^{(m-1)} - \alpha_{iq_{m-1}}^\varepsilon M_{q_1 \dots q_{m-2}}^{(m-2)} \right\rangle, \\
\hat{n}_{iq_1 \dots q_{m-1}}^{(m)} &= \frac{1}{m!} \sum_{\mathcal{P}(q)} \left\langle C_{iq_{m-1} k q_{m-2}}^\varepsilon \hat{N}_{kq_1 \dots q_{m-3}}^{(m-2)} + C_{iq_{m-1} kl}^\varepsilon \hat{N}_{q_1 \dots q_{m-2}, l}^{(m-1)} - \beta_{iq_{m-1}}^\varepsilon W_{q_1 \dots q_{m-2}}^{(m-2)} \right\rangle, \\
m_{q_1 \dots q_m}^{(m)} &= \frac{1}{m!} \sum_{\mathcal{P}(q)} \left\langle K_{q_m q_1}^\varepsilon M_{q_2 \dots q_{m-1}}^{(m-2)} + K_{q_m j}^\varepsilon M_{q_1 \dots q_{m-1}, j}^{(m-1)} \right\rangle, \\
w_{q_1 \dots q_m}^{(m)} &= \frac{1}{m!} \sum_{\mathcal{P}(q)} \left\langle D_{q_m q_1}^\varepsilon W_{q_2 \dots q_{m-1}}^{(m-2)} + D_{q_m j}^\varepsilon W_{q_1 \dots q_{m-1}, j}^{(m-1)} \right\rangle. \tag{58}
\end{aligned}$$

The perturbation functions characterizing the *down-scaling* relations (12), (13), and (14) are obtained by the solution of the previously defined cells problems, derived by imposing the normalization conditions (15). According to Bakhvalov and Panasenko (1984) and Smyshlyaev and Cherednichenko (2000), the constants (54) and (58) are determined by imposing that the non-homogeneous terms in equations (55), (51), (52), (53), (56) and (57) (associated to the auxiliary body forces (Bacigalupo, 2014), heat and mass sources) possess vanishing mean values over the unit cell \mathcal{Q} . This implies the \mathcal{Q} -periodicity of the perturbations functions $N_{kpq}^{(m)}$, $\tilde{N}_{kq}^{(m)}$, $\hat{N}_{kq}^{(m)}$, $M_q^{(m)}$, $W_q^{(m)}$, and then the continuity and regularity of the microscopic fields (micro-displacements, micro-temperature and micro-concentration) at the interface between adjacent cells are guaranteed.

A.2 Averaged field equation of infinite order and its formal solution

Using the cell problems (21), (22), (55), (51), (52), (53), (56) and (57) together with the constants definitions (23), (54) and (58) into the microscopic field equations (18), (19) and (20), the averaged equations of infinite order are derived:

$$\begin{aligned}
&n_{ipq_1 q_2}^{(2)} \frac{\partial^2 U_p}{\partial x_{q_1} \partial x_{q_2}} + \tilde{n}_{iq_1}^{(2)} \frac{\partial \Theta}{\partial x_{q_1}} + \hat{n}_{iq_1}^{(2)} \frac{\partial \Upsilon}{\partial x_{q_1}} + \sum_{n=0}^{+\infty} \varepsilon^{n+1} \sum_{|q|=n+3} n_{ipq}^{(n+3)} \frac{\partial^{n+3} U_p}{\partial x_q} \\
&+ \sum_{n=0}^{+\infty} \varepsilon^{n+1} \sum_{|q|=n+2} \tilde{n}_{iq}^{(n+2)} \frac{\partial^{n+2} \Theta}{\partial x_q} + \sum_{n=0}^{+\infty} \varepsilon^{n+1} \sum_{|q|=n+2} \hat{n}_{iq}^{(n+2)} \frac{\partial^{n+2} \Upsilon}{\partial x_q} + b_i = 0 \tag{59}
\end{aligned}$$

$$m_{q_1 q_2}^{(2)} \frac{\partial^2 \Theta}{\partial x_{q_1} \partial x_{q_2}} + \sum_{n=0}^{+\infty} \varepsilon^{n+1} \sum_{|q|=n+3} m_q^{(n+3)} \frac{\partial^{n+3} \Theta}{\partial x_q} + r = 0, \tag{60}$$

$$w_{q_1 q_2}^{(2)} \frac{\partial^2 \Upsilon}{\partial x_{q_1} \partial x_{q_2}} + \sum_{n=0}^{+\infty} \varepsilon^{n+1} \sum_{|q|=n+3} w_q^{(n+3)} \frac{\partial^{n+3} \Upsilon}{\partial x_q} + s = 0, \tag{61}$$

where q is a multi-index, $\partial^{n+j}(\cdot)/\partial x_q = \partial^{n+j}(\cdot)/\partial x_{q_1} \cdots \partial x_{q_{n+j}}$ with $j \in \mathbb{N}$, $n_{ipq}^{(n+3)} = n_{ipq_1 \cdots q_{n+3}}$, $\tilde{n}_{iq}^{(n+2)} = \tilde{n}_{iq_1 \cdots q_{n+2}}$, $\hat{n}_{iq}^{(n+2)} = \hat{n}_{iq_1 \cdots q_{n+2}}$, $m_q^{(n+3)} = m_{q_1 \cdots q_{n+3}}^{(n+3)}$ and $w_q^{(n+3)} = w_{q_1 \cdots q_{n+3}}^{(n+3)}$.

A formal solution of the averaged field equations of infinite order (59), (60) and (61) is obtained by means of an asymptotic expansion of the macroscopic fields U_i , Θ and Υ in terms of the microstructural size ε , i.e.

$$U_i(\mathbf{x}) = \sum_{j=0}^{+\infty} \varepsilon^j U_i^{(j)}(\mathbf{x}), \quad \Theta(\mathbf{x}) = \sum_{j=0}^{+\infty} \varepsilon^j \Theta^{(j)}(\mathbf{x}), \quad \Upsilon(\mathbf{x}) = \sum_{j=0}^{+\infty} \varepsilon^j \Upsilon^{(j)}(\mathbf{x}). \quad (62)$$

By substituting the series (62) into (59), (60) and (61), a sequence of equations for determining the terms of the asymptotic expansion $U_i^{(m)}$, $\Theta^{(m)}$ and $\Upsilon^{(m)}$ is obtained. At the order ε^0 , from the equation (59) we derive:

$$n_{ipq_1 q_2}^{(2)} \frac{\partial^2 U_p^{(0)}}{\partial x_{q_1} \partial x_{q_2}} + \tilde{n}_{iq_1}^{(2)} \frac{\partial \Theta^{(0)}}{\partial x_{q_1}} + \hat{n}_{iq_1}^{(2)} \frac{\partial \Upsilon^{(0)}}{\partial x_{q_1}} + b_i = 0. \quad (63)$$

whereas thermodiffusion equations (60) and (61) yield respectively

$$m_{q_1 q_2}^{(2)} \frac{\partial^2 \Theta^{(0)}}{\partial x_{q_1} \partial x_{q_2}} + r = 0, \quad w_{q_1 q_2}^{(2)} \frac{\partial^2 \Upsilon^{(0)}}{\partial x_{q_1} \partial x_{q_2}} + s = 0. \quad (64)$$

At the generic order m from (59) we obtain

$$\begin{aligned} n_{ipq_1 q_2}^{(2)} \frac{\partial^2 U_p^{(m)}}{\partial x_{q_1} \partial x_{q_2}} + \tilde{n}_{iq_1}^{(2)} \frac{\partial \Theta^{(m)}}{\partial x_{q_1}} + \hat{n}_{iq_1}^{(2)} \frac{\partial \Upsilon^{(m)}}{\partial x_{q_1}} + \sum_{r=3}^{m+2} \sum_{|q|=r} n_{ipq}^{(r)} \frac{\partial^r U_p^{(m+2-r)}}{\partial x_q} + \\ \sum_{r=3}^{m+2} \sum_{|q|=r-1} \tilde{n}_{iq}^{(r)} \frac{\partial^{r-1} \Theta^{(m+2-r)}}{\partial x_q} + \sum_{r=3}^{m+2} \sum_{|q|=r-1} \hat{n}_{iq}^{(r)} \frac{\partial^{r-1} \Upsilon^{(m+2-r)}}{\partial x_q} = 0, \end{aligned} \quad (65)$$

and (60) and (61) are given by

$$m_{q_1 q_2}^{(2)} \frac{\partial^2 \Theta^{(m)}}{\partial x_{q_1} \partial x_{q_2}} + \sum_{p=3}^{m+2} \sum_{|h|=p} m_h^{(p)} \frac{\partial^p \Theta^{(m+2-p)}}{\partial x_h} = 0, \quad (66)$$

$$w_{q_1 q_2}^{(2)} \frac{\partial^2 \Upsilon^{(m)}}{\partial x_{q_1} \partial x_{q_2}} + \sum_{p=3}^{m+2} \sum_{|h|=p} w_h^{(p)} \frac{\partial^p \Upsilon^{(m+2-p)}}{\partial x_h} = 0, \quad (67)$$

where h and q are multi-indexes. The solution of equations (63)-(67) requires that the following normalization conditions are satisfied:

$$\frac{1}{\delta L^2} \int_{\mathcal{L}} U_p^{(m)}(\mathbf{x}) d\mathbf{x} = 0, \quad \frac{1}{\delta L^2} \int_{\mathcal{L}} \Theta^{(m)}(\mathbf{x}) d\mathbf{x} = 0, \quad \frac{1}{\delta L^2} \int_{\mathcal{L}} \Upsilon^{(m)}(\mathbf{x}) d\mathbf{x} = 0, \quad (68)$$

where the \mathcal{L} -periodic domain is the same defined in previous Section as $\mathcal{L} = [0, L] \times [0, \delta L]$.

The averaged field equation (59), (60) and (61) (or alternatively the sequence of PDEs (63)-(67)), obtained by means of the proposed rigorous asymptotic procedure, are used in Sec. 4 of the

text of the paper for deriving the field equation of the first order (Cauchy) homogeneous continuum equivalent to the considered periodic thermodiffusive material.

The approximation of the average field equations (59)-(61) yielded by solution of homogenized differential problems of generic order m (65) is more accurate with respect to that obtained by the assumption (24). This implies also a more precise approximation of the solution of the microscopic field equation (7)-(8) by means of the down-scaling relation (18), (19) and (20) involving the macroscopic field (62). As it is explained for periodic elastic composites in Peerlings and Fleck (2004) and Bacigalupo and Gambarotta (2012), the truncation of the average equations of infinite order (59)-(61) at a generic order m with the aim to derive higher order field equations for generalized thermodiffusive continua may lead to problems in which the symmetries of the higher order elastic and thermodiffusive constants is not guaranteed. Moreover a loss of ellipticity of the governing equations can be observed. Asymptotic-variational homogenization techniques similar to those illustrated in Smyshlyaev and Cherednichenko (2000) and Bacigalupo and Gambarotta (2012) represent an appropriate and powerful tool in order to avoid these problems. The generalization of these methods to the case of elastic materials in presence of thermodiffusion is still missing in literature.

B Symmetry and positive definiteness of elastic and thermodiffusive tensors

In this Appendix, the symmetry properties of the tensors of components $n_{ipq_1q_2}^{(2)}$, $m_{q_1q_2}^{(2)}$, $w_{q_1q_2}^{(2)}$, and the ellipticity of the field equations (63) and (64) are demonstrated.

B.1 Symmetry and positive definiteness of tensor of components $n_{ipq_1q_2}^{(2)}$ (vs. $C_{iq_2pq_1}$)

Let us consider the cell problem $(21)_1$, remembering that $n_{ipq_1}^{(1)} = 0$, it becomes

$$\left(C_{ijkl}^m N_{kpq_1,l}^{(1)} \right)_{,j} + C_{ijpq_1}^m = 0, \quad (69)$$

where C_{ijkl}^m are \mathcal{Q} -periodic functions. The weak form of equation (69), using $N_{riq_2}^{(1)}$ as \mathcal{Q} -periodic test function, is given by

$$\left\langle \left(C_{ijkl}^m N_{kpq_1,l}^{(1)} + C_{ijpq_1}^m \right)_{,j} N_{riq_2}^{(1)} \right\rangle = 0, \quad (70)$$

applying the divergence theorem to (70), and remembering that for the \mathcal{Q} -periodicity of C_{ijkl}^m and $N_{riq_2}^{(1)}$ the path integrals evaluated on the boundary of the unit cell \mathcal{Q} vanish, we obtain:

$$\left\langle \left(C_{ijkl}^m N_{kpq_1,l}^{(1)} + C_{ijpq_1}^m \right) N_{riq_2,j}^{(1)} \right\rangle = 0. \quad (71)$$

Using the result (71), expression (54)₁ can be written in the equivalent form:

$$\begin{aligned}
n_{ipq_1q_2}^{(2)} &= \frac{1}{2} \left\langle \left(C_{iq_2pq_1}^\varepsilon + C_{iq_2kl}^\varepsilon N_{kpq_1,l}^{(1)} \right) + \left(C_{iq_1pq_2}^\varepsilon + C_{iq_1kl}^\varepsilon N_{kpq_2,l}^{(1)} \right) \right\rangle \\
&= \frac{1}{2} \left\langle C_{iq_2pq_1}^\varepsilon + C_{iq_2kl}^\varepsilon N_{kpq_1,l}^{(1)} + \left(C_{ijkl}^m N_{kpq_1,l}^{(1)} + C_{ijpq_1}^m \right) N_{riq_2,j}^{(1)} + \right. \\
&\quad \left. C_{iq_1pq_2}^\varepsilon + C_{iq_1kl}^\varepsilon N_{kpq_2,l}^{(1)} + \left(C_{rjkl}^m N_{kpq_2,l}^{(1)} + C_{rjpq_2}^m \right) N_{riq_1,j}^{(1)} \right\rangle \\
&= \frac{1}{2} \left[\frac{1}{4} \left\langle C_{rjkl}^m \left(N_{riq_2,j}^{(1)} + \delta_{ri} \delta_{jq_2} + N_{rq_2i,j}^{(1)} + \delta_{rq_2} \delta_{ij} \right) \cdot \right. \right. \\
&\quad \left. \left(N_{kpq_1,l}^{(1)} + \delta_{kp} \delta_{lq_1} + N_{kq_1p,l}^{(1)} + \delta_{kq_1} \delta_{lp} \right) \right\rangle + \\
&\quad \frac{1}{4} \left\langle C_{rjkl}^m \left(N_{riq_1,j}^{(1)} + \delta_{ri} \delta_{jq_1} + N_{rq_1i,j}^{(1)} + \delta_{rq_1} \delta_{ij} \right) \cdot \right. \\
&\quad \left. \left(N_{kpq_2,l}^{(1)} + \delta_{kp} \delta_{lq_2} + N_{kq_2p,l}^{(1)} + \delta_{kq_2} \delta_{lp} \right) \right\rangle \right], \tag{72}
\end{aligned}$$

as a consequence, we can observe that:

$$n_{ipq_1q_2}^{(2)} = \frac{1}{2} (C_{iq_2pq_1} + C_{iq_1pq_2}), \tag{73}$$

where the components $C_{iq_2pq_1}$ of the overall elastic tensor take the form:

$$C_{iq_2pq_1} = \frac{1}{4} \left\langle C_{rjkl}^m \left(N_{riq_2,j}^{(1)} + \delta_{ri} \delta_{jq_2} + N_{rq_2i,j}^{(1)} + \delta_{rq_2} \delta_{ij} \right) \cdot \left(N_{kpq_1,l}^{(1)} + \delta_{kp} \delta_{lq_1} + N_{kq_1p,l}^{(1)} + \delta_{kq_1} \delta_{lp} \right) \right\rangle, \tag{74}$$

Observing expression (74), it is easy to deduce that the tensor of components $C_{iq_2pq_1}$ is symmetric and positive definite.

B.2 Symmetry and positive definiteness of tensors of components $m_{q_1q_2}^{(2)}$ and $w_{q_1q_2}^{(2)}$ (vs. $K_{q_1q_2}$ and $D_{q_1q_2}$)

Remembering that $m_{q_1}^{(1)} = 0$, the cell problems (22)₁, possesses the form

$$\left(K_{ij}^m M_{q_1,j}^{(1)} \right)_{,i} + K_{iq_1}^m = 0 \tag{75}$$

where K_{ij}^m are \mathcal{Q} -periodic functions. The weak form of equation (75), using $M_{q_2}^{(1)}$ as \mathcal{Q} -periodic test function, is given by

$$\left\langle \left(K_{ij}^m M_{q_1,j}^{(1)} + K_{iq_1}^m \right)_{,i} M_{q_2}^{(1)} \right\rangle = 0, \tag{76}$$

applying the divergence theorem to (76), and remembering that for the \mathcal{Q} -periodicity of K_{ij}^m and $M_{q_2}^{(1)}$ the path integrals evaluated on the boundary of the unit cell \mathcal{Q} vanish, we obtain:

$$\left\langle \left(K_{ij}^m M_{q_1,j}^{(1)} + K_{iq_1}^m \right) M_{q_2,i}^{(1)} \right\rangle = 0. \tag{77}$$

Using the result (77), expression (54)₍₄₎ can be written in the equivalent form:

$$\begin{aligned}
m_{q_1 q_2}^{(2)} &= \frac{1}{2} \left\langle (K_{q_2 q_1}^m + K_{q_1 j}^m M_{q_2, j}^{(1)}) + (K_{q_1 q_2}^m + K_{q_2 j}^m M_{q_1, j}^{(1)}) \right\rangle \\
&= \frac{1}{2} \left\langle K_{q_2 q_1}^m + K_{q_1 j}^m M_{q_2, j}^{(1)} + (K_{ij}^m M_{q_1, j}^{(1)} + K_{iq_1}^m) M_{q_2, i}^{(1)} + \right. \\
&\quad \left. K_{q_1 q_2}^m + K_{q_2 j}^m M_{q_1, j}^{(1)} + (K_{ij}^m M_{q_2, j}^{(1)} + K_{iq_2}^m) M_{q_1, i}^{(1)} \right\rangle \\
&= \frac{1}{2} \left[\left\langle K_{ij}^m (M_{q_2, i}^{(1)} + \delta_{iq_2}) (M_{q_1, j}^{(1)} + \delta_{q_1 j}) \right\rangle + \right. \\
&\quad \left. \left\langle K_{ji}^m (M_{q_1, i}^{(1)} + \delta_{iq_1}) (M_{q_2, j}^{(1)} + \delta_{q_2 j}) \right\rangle \right] \\
&= \left\langle K_{ij}^m (M_{q_2, i}^{(1)} + \delta_{iq_2}) (M_{q_1, j}^{(1)} + \delta_{q_1 j}) \right\rangle
\end{aligned} \tag{78}$$

as a consequence, we can observe that $m_{q_1 q_2}^{(2)} = K_{q_1 q_2}$, i.e.

$$K_{q_1 q_2} = \left\langle K_{ij}^m (M_{q_2, i}^{(1)} + \delta_{iq_2}) (M_{q_1, j}^{(1)} + \delta_{q_1 j}) \right\rangle. \tag{79}$$

Observing expression (79), it is easy to deduce that the tensor of components $K_{q_1 q_2}$ is symmetric and positive definite. Since the equations of heat and mass diffusion possess an identical form, the components of the tensors $K_{q_1 q_2}$ and $D_{q_1 q_2}$ have the same properties, and then the results obtained for the components of the overall heat conduction tensor can be extended to the case of the overall mass diffusion tensor of components $D_{q_1 q_2}$. These components are given by the following expression:

$$D_{q_1 q_2} = \left\langle D_{ij}^m (W_{q_2, i}^{(1)} + \delta_{iq_2}) (W_{q_1, j}^{(1)} + \delta_{q_1 j}) \right\rangle. \tag{80}$$

C Overall elastic and thermodiffusive constants for bi-phase isotropic layered materials

In this Appendix the explicit expressions for the overall elastic and thermodiffusive constant of a bi-phase layered material with isotropic phases are reported. The components of the overall elastic tensor take the form:

$$\begin{aligned}
C_{1111} &= \frac{-\zeta^2 \tilde{E}_a \tilde{E}_b + \zeta [(\tilde{E}_a \tilde{\nu}_b)^2 - 2\tilde{E}_a \tilde{\nu}_a \tilde{E}_b \tilde{\nu}_b + (\tilde{E}_b \tilde{\nu}_a)^2 - (\tilde{E}_a)^2 - (\tilde{E}_b)^2] - \tilde{E}_a \tilde{E}_b}{(\zeta + 1) [\zeta (\tilde{E}_b (\tilde{\nu}_a)^2 - \tilde{E}_b) + \tilde{E}_a (\tilde{\nu}_b)^2 - \tilde{E}_a]}; \\
C_{2222} &= -\frac{(\zeta + 1) \tilde{E}_a \tilde{E}_b}{\zeta (\tilde{E}_b (\tilde{\nu}_a)^2 - \tilde{E}_b) + \tilde{E}_a (\tilde{\nu}_b)^2 - \tilde{E}_a}; \\
C_{1212} &= \frac{(\zeta + 1) \tilde{E}_a \tilde{E}_b}{2 [\tilde{E}_a + \tilde{E}_a \tilde{\nu}_b + \zeta (\tilde{E}_b \tilde{\nu}_a + \tilde{E}_b)]}; \\
C_{1122} &= -\frac{\tilde{E}_a \tilde{E}_b (\tilde{\nu}_b + \zeta \tilde{\nu}_a)}{\zeta (\tilde{E}_b (\tilde{\nu}_a)^2 - \tilde{E}_b) + \tilde{E}_a (\tilde{\nu}_b)^2 - \tilde{E}_a}.
\end{aligned} \tag{81}$$

The components of the overall thermal dilatation tensor and diffusive expansion tensor are respectively given by

$$\begin{aligned}\alpha_{11} &= \frac{A_{11}\alpha^a - B_{11}\alpha^a}{\Delta_{11}}; \\ \alpha_{22} &= \frac{\zeta(\tilde{E}_b(\tilde{\nu}_a)^2 - \tilde{E}_b)\alpha^a + \tilde{E}_a((\tilde{\nu}_b)^2 - 1)\alpha^b}{\zeta\tilde{E}_b((\tilde{\nu}_a)^2 - 1) + \tilde{E}_a((\tilde{\nu}_b)^2 - 1)};\end{aligned}\quad (82)$$

$$\begin{aligned}\beta_{11} &= \frac{A_{11}\beta^a - B_{11}\beta^a}{\Delta_{11}}; \\ \beta_{22} &= \frac{\zeta(\tilde{E}_b(\tilde{\nu}_a)^2 - \tilde{E}_b)\beta^a + \tilde{E}_a((\tilde{\nu}_b)^2 - 1)\beta^b}{\zeta\tilde{E}_b((\tilde{\nu}_a)^2 - 1) + \tilde{E}_a((\tilde{\nu}_b)^2 - 1)};\end{aligned}\quad (83)$$

where:

$$\begin{aligned}A_{11} &= \zeta^2[\tilde{E}_b(\tilde{\nu}_a)^2 - \tilde{E}_b] + \zeta[\tilde{E}_a(\tilde{\nu}_b)^2 - \tilde{E}_b\tilde{\nu}_b + \tilde{E}_b\tilde{\nu}_b(\tilde{\nu}_a)^2 + \tilde{E}_a\tilde{\nu}_a - \tilde{E}_a\tilde{\nu}_a(\tilde{\nu}_b)^2 - \tilde{E}_a]; \\ B_{11} &= \zeta[\tilde{E}_a\tilde{\nu}_a(\tilde{\nu}_b)^2 - \tilde{E}_b + \tilde{E}_b(\tilde{\nu}_a)^2 + \tilde{E}_b\tilde{\nu}_b - \tilde{E}_b\tilde{\nu}_b(\tilde{\nu}_a)^2 - \tilde{E}_a\tilde{\nu}_a] + \tilde{E}_a(\tilde{\nu}_b)^2 - \tilde{E}_a; \\ \Delta_{11} &= (\zeta + 1)[\zeta\tilde{E}_b((\tilde{\nu}_a)^2 - 1) + \tilde{E}_a((\tilde{\nu}_b)^2 - 1)].\end{aligned}\quad (84)$$

Finally, the components of the overall heat conduction and mass diffusion tensors become

$$K_{11} = \frac{K^b - \zeta K^a}{\zeta + 1}, \quad K_{22} = \frac{(\zeta + 1)K^a K^b}{K^a + \zeta K^b}; \quad (85)$$

$$D_{11} = \frac{D^b - \zeta D^a}{\zeta + 1}, \quad D_{22} = \frac{(\zeta + 1)D^a D^b}{D^a + \zeta D^b}. \quad (86)$$

D Down-scaling relations vs cells problems

In this Appendix, we provide more details regarding the structure of the down-scaling relations (12), (13) and (14) and of the related cells problems. Following the approaches proposed by Bensoussan et al. (1978); Bakhvalov and Panasenko (1984); Allaire (1992); Boutin and Auriault (1993); Meguid and Kalamkarov (1994) and Boutin (1996), the microscopic fields can be represented through an asymptotic expansion in the general form:

$$u_h\left(\mathbf{x}, \frac{\mathbf{x}}{\varepsilon}\right) = \sum_{l=1}^{+\infty} \varepsilon^l u_h^{(l)}\left(\mathbf{x}, \frac{\mathbf{x}}{\varepsilon}\right) = u_h^{(0)}\left(\mathbf{x}, \frac{\mathbf{x}}{\varepsilon}\right) + \varepsilon u_h^{(1)}\left(\mathbf{x}, \frac{\mathbf{x}}{\varepsilon}\right) + \varepsilon^2 u_h^{(2)}\left(\mathbf{x}, \frac{\mathbf{x}}{\varepsilon}\right) + \dots, \quad (87)$$

$$\theta\left(\mathbf{x}, \frac{\mathbf{x}}{\varepsilon}\right) = \sum_{l=1}^{+\infty} \varepsilon^l \theta^{(l)}\left(\mathbf{x}, \frac{\mathbf{x}}{\varepsilon}\right) = \theta^{(0)}\left(\mathbf{x}, \frac{\mathbf{x}}{\varepsilon}\right) + \varepsilon \theta^{(1)}\left(\mathbf{x}, \frac{\mathbf{x}}{\varepsilon}\right) + \varepsilon^2 \theta^{(2)}\left(\mathbf{x}, \frac{\mathbf{x}}{\varepsilon}\right) + \dots, \quad (88)$$

$$\eta\left(\mathbf{x}, \frac{\mathbf{x}}{\varepsilon}\right) = \sum_{l=1}^{+\infty} \varepsilon^l \eta^{(l)}\left(\mathbf{x}, \frac{\mathbf{x}}{\varepsilon}\right) = \eta^{(0)}\left(\mathbf{x}, \frac{\mathbf{x}}{\varepsilon}\right) + \varepsilon \eta^{(1)}\left(\mathbf{x}, \frac{\mathbf{x}}{\varepsilon}\right) + \varepsilon^2 \eta^{(2)}\left(\mathbf{x}, \frac{\mathbf{x}}{\varepsilon}\right) + \dots. \quad (89)$$

Substituting expressions (87), (88) and (89) into the microscopic field equations (7), (8), and remembering the property $\frac{\partial f}{\partial x_j}(\mathbf{x}, \boldsymbol{\xi} = \frac{\mathbf{x}}{\varepsilon}) = \left(\frac{\partial f}{\partial x_j} + \frac{1}{\varepsilon} \frac{\partial f}{\partial \xi_j}\right)_{\boldsymbol{\xi}=\mathbf{x}/\varepsilon} = \left(\frac{\partial f}{\partial x_j} + \frac{f_{,j}}{\varepsilon}\right)_{\boldsymbol{\xi}=\mathbf{x}/\varepsilon}$, we obtain

$$\begin{aligned} & \varepsilon^{-2} \left(C_{ijhl}^\varepsilon u_{h,l}^{(0)} \right)_{,j} + \varepsilon^{-1} \left\{ \left[C_{ijhl}^\varepsilon \left(\frac{\partial u_h^{(0)}}{\partial x_l} + u_{h,l}^{(1)} \right) \right]_{,j} + \left(C_{ijhl}^\varepsilon u_{h,l}^{(0)} \right)_{,j} - \left(\alpha_{ij}^\varepsilon \theta^{(0)} \right)_{,j} - \left(\beta_{ij}^\varepsilon \eta^{(0)} \right)_{,j} \right\} \\ & + \varepsilon^0 \left\{ \left[C_{ijhl}^\varepsilon \left(\frac{\partial u_h^{(1)}}{\partial x_l} + u_{h,l}^{(2)} \right) \right]_{,j} + \frac{\partial}{\partial x_j} \left[C_{ijhl}^\varepsilon \left(\frac{\partial u_h^{(0)}}{\partial x_l} + u_{h,l}^{(1)} \right) \right] - \left(\alpha_{ij}^\varepsilon \theta^{(1)} \right)_{,j} - \frac{\partial}{\partial x_j} \left(\alpha_{ij}^\varepsilon \theta^{(0)} \right) \right. \\ & - \left(\beta_{ij}^\varepsilon \eta^{(1)} \right)_{,j} - \frac{\partial}{\partial x_j} \left(\beta_{ij}^\varepsilon \eta^{(0)} \right) \left. \right\} + \varepsilon \left\{ \left[C_{ijhl}^\varepsilon \left(\frac{\partial u_h^{(2)}}{\partial x_l} + u_{h,l}^{(3)} \right) \right]_{,j} + \frac{\partial}{\partial x_j} \left[C_{ijhl}^\varepsilon \left(\frac{\partial u_h^{(1)}}{\partial x_l} + u_{h,l}^{(2)} \right) \right] \right. \\ & - \left(\alpha_{ij}^\varepsilon \theta^{(2)} \right)_{,j} - \frac{\partial}{\partial x_j} \left(\alpha_{ij}^\varepsilon \theta^{(1)} \right) - \left(\beta_{ij}^\varepsilon \eta^{(2)} \right)_{,j} - \frac{\partial}{\partial x_j} \left(\beta_{ij}^\varepsilon \eta^{(1)} \right) \left. \right\} + \dots + b_i = 0, \quad i = 1, 2, \end{aligned} \quad (90)$$

$$\begin{aligned} & \varepsilon^{-2} \left(K_{ij}^\varepsilon \theta_{,j}^{(0)} \right)_{,i} + \varepsilon^{-1} \left\{ \left[K_{ij}^\varepsilon \left(\frac{\partial \theta^{(0)}}{\partial x_j} + \theta_{,j}^{(1)} \right) \right]_{,i} + \frac{\partial}{\partial x_i} \left(K_{ij}^\varepsilon \theta_{,j}^{(0)} \right) \right\} \\ & + \varepsilon^0 \left\{ \left[K_{ij}^\varepsilon \left(\frac{\partial \theta^{(1)}}{\partial x_j} + \theta_{,j}^{(2)} \right) \right]_{,i} + \frac{\partial}{\partial x_i} \left[K_{ij}^\varepsilon \left(\frac{\partial \theta^{(0)}}{\partial x_j} + \theta_{,j}^{(1)} \right) \right] \right\} \\ & + \varepsilon \left\{ \left[K_{ij}^\varepsilon \left(\frac{\partial \theta^{(2)}}{\partial x_j} + \theta_{,j}^{(3)} \right) \right]_{,i} + \frac{\partial}{\partial x_i} \left[K_{ij}^\varepsilon \left(\frac{\partial \theta^{(1)}}{\partial x_j} + \theta_{,j}^{(2)} \right) \right] \right\} + \dots + r = 0, \end{aligned} \quad (91)$$

$$\begin{aligned} & \varepsilon^{-2} \left(D_{ij}^\varepsilon \eta_{,j}^{(0)} \right)_{,i} + \varepsilon^{-1} \left\{ \left[D_{ij}^\varepsilon \left(\frac{\partial \eta^{(0)}}{\partial x_j} + \eta_{,j}^{(1)} \right) \right]_{,i} + \frac{\partial}{\partial x_i} \left(D_{ij}^\varepsilon \eta_{,j}^{(0)} \right) \right\} \\ & + \varepsilon^0 \left\{ \left[D_{ij}^\varepsilon \left(\frac{\partial \eta^{(1)}}{\partial x_j} + \eta_{,j}^{(2)} \right) \right]_{,i} + \frac{\partial}{\partial x_i} \left[D_{ij}^\varepsilon \left(\frac{\partial \eta^{(0)}}{\partial x_j} + \eta_{,j}^{(1)} \right) \right] \right\} \\ & + \varepsilon \left\{ \left[D_{ij}^\varepsilon \left(\frac{\partial \eta^{(2)}}{\partial x_j} + \eta_{,j}^{(3)} \right) \right]_{,i} + \frac{\partial}{\partial x_i} \left[D_{ij}^\varepsilon \left(\frac{\partial \eta^{(1)}}{\partial x_j} + \eta_{,j}^{(2)} \right) \right] \right\} + \dots + s = 0. \end{aligned} \quad (92)$$

At the order ε^{-2} from equation (90) we derive:

$$\left(C_{ijhl}^\varepsilon u_{h,l}^{(0)} \right)_{,j} = f_i^{(0)}(\mathbf{x}), \quad (93)$$

whereas from heat conduction and mass diffusion equations (91) and (92) we get respectively:

$$\left(K_{ij}^\varepsilon \theta_{,j}^{(0)} \right)_{,i} = g^{(0)}(\mathbf{x}), \quad \left(D_{ij}^\varepsilon \eta_{,j}^{(0)} \right)_{,i} = h^{(0)}(\mathbf{x}). \quad (94)$$

The interface conditions (9)-(11), expressed with respect to $\boldsymbol{\xi}$, become:

$$\llbracket u_h^{(0)} \rrbracket \Big|_{\boldsymbol{\xi} \in \Sigma_1} = 0, \quad \left[\left[C_{ijhl}^\varepsilon u_{h,l}^{(0)} n_j \right] \right] \Big|_{\boldsymbol{\xi} \in \Sigma_1} = 0, \quad (95)$$

$$\llbracket \theta^{(0)} \rrbracket \Big|_{\boldsymbol{\xi} \in \Sigma_1} = 0, \quad \left[\left[K_{ij}^\varepsilon \theta_{,j}^{(0)} n_i \right] \right] \Big|_{\boldsymbol{\xi} \in \Sigma_1} = 0, \quad (96)$$

$$\llbracket \eta^{(0)} \rrbracket \Big|_{\boldsymbol{\xi} \in \Sigma_1} = 0, \quad \left[\left[D_{ij}^\varepsilon \eta_{,j}^{(0)} n_i \right] \right] \Big|_{\boldsymbol{\xi} \in \Sigma_1} = 0, \quad (97)$$

where Σ_1 is the representation of the interface Σ between two different phases of the material in the non-dimensional space of the variable $\boldsymbol{\xi}$.

At the order ε^{-1} equation (90) yields

$$\left[C_{ijhl}^\varepsilon \left(\frac{\partial u_h^{(0)}}{\partial x_l} + u_{h,l}^{(1)} \right) \right]_{,j} + \frac{\partial}{\partial x_j} \left(C_{ijhl}^\varepsilon u_{h,l}^{(0)} \right)_{,j} - \left(\alpha_{ij}^\varepsilon \theta^{(0)} \right)_{,j} - \left(\beta_{ij}^\varepsilon \eta^{(0)} \right)_{,j} = f_i^{(1)}(\mathbf{x}), \quad (98)$$

at the same order, from equations (91) and (92) we obtain:

$$\left[K_{ij}^\varepsilon \left(\frac{\partial \theta^{(0)}}{\partial x_j} + \theta_{,j}^{(1)} \right) \right]_{,i} + \frac{\partial}{\partial x_i} \left(K_{ij}^\varepsilon \theta_{,j}^{(0)} \right) = g^{(1)}(\mathbf{x}), \quad (99)$$

$$\left[D_{ij}^\varepsilon \left(\frac{\partial \eta^{(0)}}{\partial x_j} + \eta_{,j}^{(1)} \right) \right]_{,i} + \frac{\partial}{\partial x_i} \left(D_{ij}^\varepsilon \eta_{,j}^{(0)} \right) = h^{(1)}(\mathbf{x}), \quad (100)$$

and the interface conditions are given by

$$\llbracket u_h^{(1)} \rrbracket \Big|_{\boldsymbol{\xi} \in \Sigma_1} = 0; \quad \left[\left[\left(C_{ijhl}^\varepsilon \left(\frac{\partial u_h^{(0)}}{\partial x_l} + u_{h,l}^{(1)} \right) - \alpha_{ij}^\varepsilon \theta^{(0)} - \beta_{ij}^\varepsilon \eta^{(0)} \right) n_j \right] \right] \Big|_{\boldsymbol{\xi} \in \Sigma_1} = 0, \quad (101)$$

$$\llbracket \theta^{(1)} \rrbracket \Big|_{\boldsymbol{\xi} \in \Sigma_1} = 0; \quad \left[\left[K_{ij}^\varepsilon \left(\theta_{,j}^{(1)} + \frac{\partial \theta^{(0)}}{\partial x_j} \right) n_i \right] \right] \Big|_{\boldsymbol{\xi} \in \Sigma_1} = 0, \quad (102)$$

$$\llbracket \eta^{(1)} \rrbracket \Big|_{\boldsymbol{\xi} \in \Sigma_1} = 0; \quad \left[\left[D_{ij}^\varepsilon \left(\eta_{,j}^{(1)} + \frac{\partial \eta^{(0)}}{\partial x_j} \right) n_i \right] \right] \Big|_{\boldsymbol{\xi} \in \Sigma_1} = 0. \quad (103)$$

At the order ε^0 , the cells problems associate to equation (90) assume the form:

$$\begin{aligned} & \left[C_{ijhl}^\varepsilon \left(\frac{\partial u_h^{(1)}}{\partial x_l} + u_{h,l}^{(2)} \right) \right]_{,j} + \frac{\partial}{\partial x_j} \left[C_{ijhl}^\varepsilon \left(\frac{\partial u_h^{(0)}}{\partial x_l} + u_{h,l}^{(1)} \right) \right] \\ & - \left(\alpha_{ij}^\varepsilon \theta^{(1)} \right)_{,j} - \frac{\partial}{\partial x_j} \left(\alpha_{ij}^\varepsilon \theta^{(0)} \right) - \left(\beta_{ij}^\varepsilon \eta^{(1)} \right)_{,j} - \frac{\partial}{\partial x_j} \left(\beta_{ij}^\varepsilon \eta^{(0)} \right) = f_i^{(2)}(\mathbf{x}), \end{aligned} \quad (104)$$

whereas the cells problems corresponding to equations (91) and (92) are:

$$\left[K_{ij}^\varepsilon \left(\frac{\partial \theta^{(1)}}{\partial x_j} + \theta_{,j}^{(2)} \right) \right]_{,i} + \frac{\partial}{\partial x_i} \left[K_{ij}^\varepsilon \left(\frac{\partial \theta^{(0)}}{\partial x_j} + \theta_{,j}^{(1)} \right) \right] = g^{(2)}(\mathbf{x}), \quad (105)$$

$$\left[D_{ij}^\varepsilon \left(\frac{\partial \eta^{(1)}}{\partial x_j} + \eta_{,j}^{(2)} \right) \right]_{,i} + \frac{\partial}{\partial x_i} \left[D_{ij}^\varepsilon \left(\frac{\partial \eta^{(0)}}{\partial x_j} + \eta_{,j}^{(1)} \right) \right] = h^{(2)}(\mathbf{x}), \quad (106)$$

and the interface conditions assume the form:

$$\llbracket u_h^{(2)} \rrbracket \Big|_{\boldsymbol{\xi} \in \Sigma_1} = 0, \quad \left[\left[\left(C_{ijhl}^\varepsilon \left(\frac{\partial u_h^{(1)}}{\partial x_l} + u_{h,l}^{(2)} \right) - \alpha_{ij}^\varepsilon \theta^{(1)} - \beta_{ij}^\varepsilon \eta^{(1)} \right) n_j \right] \right] \Big|_{\boldsymbol{\xi} \in \Sigma_1} = 0, \quad (107)$$

$$\llbracket \theta^{(2)} \rrbracket \Big|_{\boldsymbol{\xi} \in \Sigma_1} = 0, \quad \left[\left[K_{ij}^\varepsilon \left(\theta_{,j}^{(2)} + \frac{\partial \theta^{(1)}}{\partial x_j} \right) n_i \right] \right] \Big|_{\boldsymbol{\xi} \in \Sigma_1} = 0, \quad (108)$$

$$\llbracket \eta^{(2)} \rrbracket \Big|_{\boldsymbol{\xi} \in \Sigma_1} = 0, \quad \left[\left[D_{ij}^\varepsilon \left(\eta_{,j}^{(2)} + \frac{\partial \eta^{(1)}}{\partial x_j} \right) n_i \right] \right] \Big|_{\boldsymbol{\xi} \in \Sigma_1} = 0. \quad (109)$$

At the order ε^{-2} , the solvability conditions in the class of the functions \mathcal{Q} -periodic with respect to the fast variable $\boldsymbol{\xi}$ implies that $f_i^{(0)}(\mathbf{x}) = g^{(0)}(\mathbf{x}) = h^{(0)}(\mathbf{x}) = 0$, then the cell problems (93)-(94) become:

$$\left(C_{ijhl}^\varepsilon u_{h,l}^{(0)} \right)_{,j} = 0, \quad \left(K_{ij}^\varepsilon \theta_{,j}^{(0)} \right)_{,i} = 0, \quad \left(D_{ij}^\varepsilon \eta_{,j}^{(0)} \right)_{,i} = 0, \quad (110)$$

as a consequence, the solution of problems (110) does not depend by the fast variable $\boldsymbol{\xi}$ and then $u_h^{(0)}(\mathbf{x}, \boldsymbol{\xi}) = U_h(\mathbf{x})$, $\theta^{(0)}(\mathbf{x}, \boldsymbol{\xi}) = \Theta(\mathbf{x})$ and $\eta^{(0)}(\mathbf{x}, \boldsymbol{\xi}) = \Upsilon(\mathbf{x})$.

At the order ε^{-1} , the solvability conditions in the class of the functions \mathcal{Q} -periodic with respect to the fast variable $\boldsymbol{\xi}$ together with the interface conditions (101)-(103) yield to

$$\langle C_{ijhl,j}^\varepsilon \rangle \frac{\partial U_h}{\partial x_l} - \langle \alpha_{ij,j}^\varepsilon \rangle \Theta^{(1)} - \langle \beta_{ij,j}^\varepsilon \rangle \Upsilon = f_i^{(1)}(\mathbf{x}), \quad (111)$$

$$\langle K_{ij,i}^\varepsilon \rangle \frac{\partial \Theta}{\partial x_j} = g^{(1)}(\mathbf{x}), \quad \langle D_{ij,i}^\varepsilon \rangle \frac{\partial \Upsilon}{\partial x_j} = h^{(1)}(\mathbf{x}). \quad (112)$$

For the \mathcal{Q} -periodicity of the functions $C_{ijhl}^\varepsilon, \alpha_{ij}^\varepsilon, \beta_{ij}^\varepsilon, K_{ij}^\varepsilon$ and D_{ij}^ε , we have $f_i^{(1)}(\mathbf{x}) = g^{(1)}(\mathbf{x}) = h^{(1)}(\mathbf{x}) = 0$, and then at this order the solution of the fields equations assumes the form:

$$u_h^{(1)}(\mathbf{x}, \boldsymbol{\xi}) = N_{hpq_1}^{(1)}(\boldsymbol{\xi}) \frac{\partial U_p}{\partial x_{q_1}} + \tilde{N}_h^{(1)}(\boldsymbol{\xi}) \Theta(\mathbf{x}) + \hat{N}_h^{(1)}(\boldsymbol{\xi}) \Upsilon(\mathbf{x}), \quad (113)$$

$$\theta^{(1)}(\mathbf{x}, \boldsymbol{\xi}) = M_{q_1}^{(1)}(\boldsymbol{\xi}) \frac{\partial \Theta}{\partial x_{q_1}}, \quad \eta^{(1)}(\mathbf{x}, \boldsymbol{\xi}) = W_{q_1}^{(1)}(\boldsymbol{\xi}) \frac{\partial \Upsilon}{\partial x_{q_1}}, \quad (114)$$

where $N_{hpq_1}^{(1)}, \tilde{N}_h^{(1)}, \hat{N}_h^{(1)}, M_{q_1}^{(1)}$ and $W_{q_1}^{(1)}$ are the same fluctuations functions introduced in Section 3. Substituting expressions (113)-(114) into the cell problems (111)-(112) and considering the interface conditions (101)-(103), we derive:

$$\left(C_{ijhl}^\varepsilon N_{hpq_1}^{(1)} \right)_{,j} + C_{ijpq_1}^\varepsilon = 0, \quad \left(C_{ijhl}^\varepsilon \tilde{N}_{h,l}^{(1)} \right)_{,j} - \alpha_{ij,j}^\varepsilon = 0, \quad \left(C_{ijhl}^\varepsilon \hat{N}_{h,l}^{(1)} \right)_{,j} - \beta_{ij,j}^\varepsilon = 0, \quad (115)$$

$$\left(K_{ij}^\varepsilon M_{q_1,j}^{(1)} \right)_{,i} + K_{iq_1,i}^\varepsilon = 0, \quad \left(D_{ij}^\varepsilon W_{q_1,j}^{(1)} \right)_{,i} + W_{iq_1,i}^\varepsilon = 0, \quad (116)$$

and then the interface conditions (101)-(103) become;

$$\llbracket N_{hpq_1}^{(1)} \rrbracket \Big|_{\boldsymbol{\xi} \in \Sigma_1} = 0, \quad \left[\left[C_{ijhl}^\varepsilon \left(N_{hpq_1,l}^{(1)} + \delta_{hp} \delta_{lq_1} \right) n_j \right] \right] \Big|_{\boldsymbol{\xi} \in \Sigma_1} = 0, \quad (117)$$

$$\llbracket \tilde{N}_h^{(1)} \rrbracket \Big|_{\boldsymbol{\xi} \in \Sigma_1} = 0, \quad \left[\left[\left(C_{ijhl}^\varepsilon \tilde{N}_{h,l}^{(1)} - \alpha_{ij}^\varepsilon \right) n_j \right] \right] \Big|_{\boldsymbol{\xi} \in \Sigma_1} = 0, \quad (118)$$

$$\llbracket \hat{N}_h^{(1)} \rrbracket \Big|_{\boldsymbol{\xi} \in \Sigma_1} = 0, \quad \left[\left[\left(C_{ijhl}^\varepsilon \hat{N}_{h,l}^{(1)} - \beta_{ij}^\varepsilon \right) n_j \right] \right] \Big|_{\boldsymbol{\xi} \in \Sigma_1} = 0, \quad (119)$$

$$\llbracket M_{q_1}^{(1)} \rrbracket \Big|_{\boldsymbol{\xi} \in \Sigma_1} = 0, \quad \left[\left[K_{ij}^\varepsilon \left(M_{q_1,j}^{(1)} + \delta_{q_1j} \right) n_i \right] \right] \Big|_{\boldsymbol{\xi} \in \Sigma_1} = 0, \quad (120)$$

$$\llbracket W_{q_1}^{(1)} \rrbracket \Big|_{\boldsymbol{\xi} \in \Sigma_1} = 0, \quad \left[\left[D_{ij}^\varepsilon \left(W_{q_1,j}^{(1)} + \delta_{q_1j} \right) n_i \right] \right] \Big|_{\boldsymbol{\xi} \in \Sigma_1} = 0. \quad (121)$$

The solution of the cell problems (115)-(116) taking into account the interface conditions (117)-(121) provides the \mathcal{Q} -periodic perturbation functions $N_{hpq_1}^{(1)}$, $\tilde{N}_h^{(1)}$, $\hat{N}_h^{(1)}$, $M_{q_1}^{(1)}$ and $W_{q_1}^{(1)}$.

Taking into account the solvability conditions in the class of the functions \mathcal{Q} -periodic with respect to the fast variable $\boldsymbol{\xi}$ and the interface conditions (107)-(109), the cell problems (104)-(106) associate to the ε^0 become:

$$\langle C_{iq_1pl}^\varepsilon + C_{ilhj}^\varepsilon N_{hpq_1,j}^{(1)} \rangle \frac{\partial^2 U_p}{\partial x_{q_1} \partial x_l} - \langle C_{ilhj}^\varepsilon \tilde{N}_{h,j}^{(1)} - \alpha_{il}^\varepsilon \rangle \frac{\partial \Theta}{\partial x_l} - \langle C_{ilhj}^\varepsilon \hat{N}_{h,j}^{(1)} - \beta_{il}^\varepsilon \rangle \frac{\partial \Upsilon}{\partial x_l} = f_i^{(2)}(\mathbf{x}), \quad (122)$$

$$\left\langle K_{ij}^\varepsilon \left(M_{q_1,j}^{(1)} + \delta_{jq_1} \right) \right\rangle \frac{\partial^2 \Theta}{\partial x_i \partial x_{q_1}} = g^{(2)}(\mathbf{x}), \quad \left\langle D_{ij}^\varepsilon \left(W_{q_1,j}^{(1)} + \delta_{jq_1} \right) \right\rangle \frac{\partial^2 \Upsilon}{\partial x_i \partial x_{q_1}} = h^{(2)}(\mathbf{x}). \quad (123)$$

these cell problems possess a solution satisfying the conditions (107)-(109) in the form:

$$u_h^{(2)}(\mathbf{x}, \boldsymbol{\xi}) = N_{hpq_1q_2}^{(2)} \frac{\partial^2 U_p}{\partial x_{q_1} \partial x_{q_2}} + \tilde{N}_{hq_1}^{(2)} \frac{\partial \Theta}{\partial x_{q_1}} + \hat{N}_{hq_1}^{(2)} \frac{\partial \Upsilon}{\partial x_{q_1}}, \quad (124)$$

$$\theta^{(2)}(\mathbf{x}, \boldsymbol{\xi}) = M_{q_1q_2}^{(2)} \frac{\partial^2 \Theta}{\partial x_{q_2} \partial x_{q_1}}, \quad \eta^{(2)}(\mathbf{x}, \boldsymbol{\xi}) = W_{q_1q_2}^{(2)} \frac{\partial^2 \Upsilon}{\partial x_{q_2} \partial x_{q_1}}, \quad (125)$$

where $N_{hpq_1q_2}^{(2)}$, $\tilde{N}_{hq_1}^{(2)}$, $\hat{N}_{hq_1}^{(2)}$, $M_{q_1q_2}^{(2)}$ and $W_{q_1q_2}^{(2)}$ are second order fluctuations functions just introduced in Section 3. As a consequence, from the cell problems (122)-(123) we derive:

$$\left(C_{ijhl}^\varepsilon N_{hpq_1q_2,l}^{(2)} \right)_{,j} + \left(C_{ijhq_2}^\varepsilon N_{hpq_1}^{(1)} \right)_{,j} + C_{iq_1pq_2}^\varepsilon + C_{iq_2hj}^\varepsilon N_{hpq_1,j}^{(1)} = \langle C_{iq_1pq_2}^\varepsilon + C_{iq_2hj}^\varepsilon N_{hpq_1,j}^{(1)} \rangle, \quad (126)$$

$$\left(C_{ijhl}^\varepsilon \tilde{N}_{hq_1,l}^{(2)} \right)_{,j} + \left(C_{ijhq_1}^\varepsilon \tilde{N}_h^{(1)} \right)_{,j} + C_{iq_1kj}^\varepsilon \tilde{N}_{h,j}^{(1)} - \left(\alpha_{ij}^\varepsilon M_{q_1}^{(1)} \right)_{,j} - \alpha_{iq_1}^\varepsilon = \langle C_{iq_1hj}^\varepsilon \tilde{N}_{h,j}^{(1)} - \alpha_{iq_1}^\varepsilon \rangle, \quad (127)$$

$$\left(C_{ijhl}^\varepsilon \hat{N}_{hq_1,l}^{(2)} \right)_{,j} + \left(C_{ijhq_1}^\varepsilon \hat{N}_h^{(1)} \right)_{,j} + C_{iq_1kj}^\varepsilon \hat{N}_{h,j}^{(1)} - \left(\beta_{ij}^\varepsilon W_{q_1}^{(1)} \right)_{,j} - \beta_{iq_1}^\varepsilon = \langle C_{iq_1hj}^\varepsilon \hat{N}_{h,j}^{(1)} - \beta_{iq_1}^\varepsilon \rangle, \quad (128)$$

$$\left(K_{ij}^\varepsilon M_{q_1q_2,j}^{(2)} \right)_{,i} + \left(K_{iq_2}^\varepsilon M_{q_1}^{(1)} \right)_{,i} + K_{iq_2}^\varepsilon \left(M_{q_1,j}^{(1)} + \delta_{jq_1} \right) = \left\langle K_{q_2j}^\varepsilon \left(M_{q_1,j}^{(1)} + \delta_{jq_1} \right) \right\rangle, \quad (129)$$

$$\left(D_{ij}^\varepsilon W_{q_1q_2,j}^{(2)} \right)_{,i} + \left(D_{iq_2}^\varepsilon W_{q_1}^{(1)} \right)_{,i} + D_{iq_2}^\varepsilon \left(W_{q_1,j}^{(1)} + \delta_{jq_1} \right) = \left\langle D_{q_2j}^\varepsilon \left(W_{q_1,j}^{(1)} + \delta_{jq_1} \right) \right\rangle, \quad (130)$$

and then the interface conditions (107)-(109) become;

$$\llbracket N_{hpq_1q_2}^{(2)} \rrbracket \Big|_{\boldsymbol{\xi} \in \Sigma_1} = 0, \quad \left[\left[\left(C_{ijhl}^\varepsilon N_{hpq_1q_2,l}^{(2)} + C_{ijhq_2}^\varepsilon N_{hpq_1}^{(1)} \right) n_j \right] \right] \Big|_{\boldsymbol{\xi} \in \Sigma_1} = 0, \quad (131)$$

$$\llbracket \tilde{N}_{hq_1}^{(2)} \rrbracket \Big|_{\boldsymbol{\xi} \in \Sigma_1} = 0, \quad \left[\left[\left(C_{ijhl}^\varepsilon \tilde{N}_{hq_1,l}^{(2)} + C_{ijhq_1}^\varepsilon \tilde{N}_h^{(1)} - \alpha_{ij}^\varepsilon M_{q_1}^{(1)} \right) n_j \right] \right] \Big|_{\boldsymbol{\xi} \in \Sigma_1} = 0, \quad (132)$$

$$\llbracket \hat{N}_{hq_1}^{(2)} \rrbracket \Big|_{\boldsymbol{\xi} \in \Sigma_1} = 0, \quad \left[\left[\left(C_{ijhl}^\varepsilon \hat{N}_{hq_1,l}^{(2)} + C_{ijhq_1}^\varepsilon \hat{N}_h^{(1)} - \beta_{ij}^\varepsilon W_{q_1}^{(1)} \right) n_j \right] \right] \Big|_{\boldsymbol{\xi} \in \Sigma_1} = 0, \quad (133)$$

$$\llbracket M_{q_1 q_2}^{(2)} \rrbracket \Big|_{\boldsymbol{\xi} \in \Sigma_1} = 0, \quad \left[\left[K_{ij}^\varepsilon \left(M_{q_1 q_2,j}^{(2)} + M_{q_1}^{(1)} \delta_{jq_2} \right) n_i \right] \right] \Big|_{\boldsymbol{\xi} \in \Sigma_1} = 0, \quad (134)$$

$$\llbracket W_{q_1 q_2}^{(2)} \rrbracket \Big|_{\boldsymbol{\xi} \in \Sigma_1} = 0, \quad \left[\left[S_{ij}^\varepsilon \left(W_{q_1 q_2,j}^{(2)} + W_{q_1}^{(1)} \delta_{jq_2} \right) n_i \right] \right] \Big|_{\boldsymbol{\xi} \in \Sigma_1} = 0. \quad (135)$$

The solution of the cell problems (126)-(130) taking into account the interface conditions (131)-(135) provides the \mathcal{Q} -periodic perturbation functions $N_{hpq_1 q_2}^{(2)}$, $\tilde{N}_{hq_1}^{(2)}$, $\hat{N}_{hq_1}^{(2)}$, $M_{q_1 q_2}^{(2)}$ and $W_{q_1 q_2}^{(2)}$.

The general procedure here reported can be applied to higher order cell problems for deriving the averaged field equations of infinite order, which assume the form:

$$\begin{aligned} & \langle C_{iq_1 pl}^\varepsilon + C_{ilhj}^\varepsilon N_{hpq_1,j}^{(1)} \rangle \frac{\partial^2 U_p}{\partial x_{q_1} \partial x_l} - \langle C_{ilhj}^\varepsilon \tilde{N}_{h,j}^{(1)} - \alpha_{il}^\varepsilon \rangle \frac{\partial \Theta}{\partial x_l} - \langle C_{ilhj}^\varepsilon \hat{N}_{h,j}^{(1)} - \beta_{il}^\varepsilon \rangle \frac{\partial \Upsilon}{\partial x_l} \\ & + \langle C_{iq_3 hq_2}^\varepsilon N_{hpq_1}^{(1)} + C_{iq_3 hl}^\varepsilon N_{hpq_1 q_2,l}^{(2)} \rangle \frac{\partial^3 U_p}{\partial x_{q_1} \partial x_{q_2} \partial x_{q_3}} + \langle C_{iq_1 hq_2}^\varepsilon \tilde{N}_h^{(1)} + C_{iq_2 hl}^\varepsilon \tilde{N}_{hq_1,l}^{(2)} - \alpha_{iq_2}^\varepsilon M_{q_1}^{(1)} \rangle \frac{\partial^2 \Theta}{\partial x_{q_1} \partial x_{q_2}} \\ & + \langle C_{iq_1 hq_2}^\varepsilon \hat{N}_h^{(1)} + C_{iq_2 hl}^\varepsilon \hat{N}_{hq_1,l}^{(2)} - \beta_{iq_2}^\varepsilon W_{q_1}^{(1)} \rangle \frac{\partial^2 \Upsilon}{\partial x_{q_1} \partial x_{q_2}} + \dots + b_i(\mathbf{x}) = 0, \end{aligned} \quad (136)$$

$$\begin{aligned} & \left\langle K_{q_2 j}^\varepsilon \left(M_{q_1,j}^{(1)} + \delta_{jq_1} \right) \right\rangle \frac{\partial^2 \Theta}{\partial x_{q_2} \partial x_{q_1}} + \left\langle K_{q_3 q_2}^\varepsilon M_{q_2}^{(1)} + K_{q_3 j}^\varepsilon M_{q_1 q_2,j}^{(2)} \right\rangle \frac{\partial^3 \Theta}{\partial x_{q_1} \partial x_{q_2} \partial x_{q_3}} \\ & + \dots + r(\mathbf{x}) = 0, \end{aligned} \quad (137)$$

$$\begin{aligned} & \left\langle D_{q_2 j}^\varepsilon \left(W_{q_1,j}^{(1)} + \delta_{jq_1} \right) \right\rangle \frac{\partial^2 \Upsilon}{\partial x_{q_2} \partial x_{q_1}} + \left\langle D_{q_3 q_2}^\varepsilon W_{q_2}^{(1)} + D_{q_3 j}^\varepsilon W_{q_1 q_2,j}^{(2)} \right\rangle \frac{\partial^3 \Upsilon}{\partial x_{q_1} \partial x_{q_2} \partial x_{q_3}} \\ & + \dots + s(\mathbf{x}) = 0. \end{aligned} \quad (138)$$

Note that applying the permutation of the saturated indexes, (136), (137) and (138) become identical to the averaged field equations derived in Appendix A. The structure of the down-scaling relations is defined by the solutions of the various cells problems associate to the different orders of the asymptotic expansion. These down-scaling relations assume the form:

$$\begin{aligned} u_h \left(\mathbf{x}, \frac{\mathbf{x}}{\varepsilon} \right) = & \left[U_h(\mathbf{x}) + \varepsilon \left(N_{hpq_1}^{(1)}(\boldsymbol{\xi}) \frac{\partial U_p(\mathbf{x})}{\partial x_{q_1}} + \tilde{N}_h^{(1)}(\boldsymbol{\xi}) \Theta(\mathbf{x}) + \hat{N}_h^{(1)}(\boldsymbol{\xi}) \Upsilon(\mathbf{x}) \right) + \right. \\ & \left. + \varepsilon^2 \left(N_{hpq_1 q_2}^{(2)}(\boldsymbol{\xi}) \frac{\partial^2 U_p(\mathbf{x})}{\partial x_{q_1} \partial x_{q_2}} + \tilde{N}_{hq_1}^{(2)}(\boldsymbol{\xi}) \frac{\partial \Theta(\mathbf{x})}{\partial x_{q_1}} + \hat{N}_{hq_1}^{(2)}(\boldsymbol{\xi}) \frac{\partial \Upsilon(\mathbf{x})}{\partial x_{q_1}} \right) + \dots \right]_{\boldsymbol{\xi}=\mathbf{x}/\varepsilon}, \end{aligned} \quad (139)$$

$$\theta \left(\mathbf{x}, \frac{\mathbf{x}}{\varepsilon} \right) = \left[\Theta(\mathbf{x}) + \varepsilon M_{q_1}^{(1)}(\boldsymbol{\xi}) \frac{\partial \Theta(\mathbf{x})}{\partial x_{q_1}} + \varepsilon^2 M_{q_1 q_2}^{(2)}(\boldsymbol{\xi}) \frac{\partial^2 \Theta(\mathbf{x})}{\partial x_{q_1} \partial x_{q_2}} + \dots \right]_{\boldsymbol{\xi}=\mathbf{x}/\varepsilon} \quad (140)$$

$$\eta \left(\mathbf{x}, \frac{\mathbf{x}}{\varepsilon} \right) = \left[\Upsilon(\mathbf{x}) + \varepsilon W_{q_1}^{(1)}(\boldsymbol{\xi}) \frac{\partial \Upsilon(\mathbf{x})}{\partial x_{q_1}} + \varepsilon^2 W_{q_1 q_2}^{(2)}(\boldsymbol{\xi}) \frac{\partial^2 \Upsilon(\mathbf{x})}{\partial x_{q_1} \partial x_{q_2}} + \dots \right]_{\boldsymbol{\xi}=\mathbf{x}/\varepsilon}. \quad (141)$$

The relations (139), (140) and (141) are identical to expressions (12), (13) and (14) introduced in Section 3 and used for developing the homogenization method illustrated in the paper.