Multiscale asymptotic homogenization analysis of thermo-diffusive composite materials

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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 mass concentration 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 multi-phase 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, multi-phase 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 (Nakao 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 multi-physics 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, multi-scale 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); Gamblin and Kroner (1989); Allaire (1992); Boutin and Auriault (1993); Meguid and Kalamkarov (1994); Boutin (1996); Andrianov et al. (2008); Tran et al. (2013)), the variational-asymptotic methods (see for example Smyshlyaev and Cherndichenko (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. Multi-scale asymptotic and computational homogenization procedures have been also proposed for the analysis of heterogeneous media in presence of multi-physics phenomena, such as thermo-mechanical (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 effects of the microstructural 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 multi-layered 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 Cherndichenko
Bacigalupo (2014) and Bacigalupo and Gambarotta (2014) is extended in order to account for the effects of the microstructures on the macroscopic temperature and mass concentration of the materials and on the stresses induced by these fields. The displacements, temperature and mass concentration at the micro- and macro-scale are related through an asymptotic expansion of the microscopic fields in terms of characteristic size $\varepsilon$ of the microstructure. This expansion depends both on the macroscopic strains, temperature and mass concentration 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, mass concentration 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 fields equations of infinite order are obtained, and their formal solution is performed by representing the macroscopic displacements, temperature and mass concentration in terms of power series. Fields 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 obtained 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 multi-scale asymptotic homogenization technique is described in Section 3, based on down-scaling relations correlating the microscopic fields to the macroscopic displacements, temperature and mass concentration. 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 fields equations of infinite order are obtained, and a solution scheme based on asymptotic expansion of the macroscopic displacements, temperature and mass concentration fields 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 continuum. The material point is identified by position vector $\mathbf{x} = x_1 e_1 + x_2 e_2$ referred to a
system of coordinates with origin at point \( O \) and orthogonal base \( \{ e_1, e_2 \} \). The periodic cell \( \mathcal{A} = [0, \varepsilon] \times [0, \delta \varepsilon] \) with characteristic size \( \varepsilon \) is illustrated in Fig. 1b. The entire periodic medium can be obtained spanning the cell \( \mathcal{A} \) by the two orthogonal vectors \( \mathbf{v}_1 = d_1 e_1 = \varepsilon e_1 \), \( \mathbf{v}_2 = d_2 e_2 = \delta \varepsilon e_2 \).

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

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

(1)

Similarly, the heat conduction tensor \( K^{(m, \varepsilon)}(\mathbf{x}) \) and the thermal dilatation tensor \( \alpha^{(m, \varepsilon)}(\mathbf{x}) \) are defined as follows

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

(2)

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

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

(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 \( \varepsilon \), 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 \( \varepsilon \).

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 \( \varepsilon \) is introduced. Two distinct scales are represented by the macroscopic (slow) variables \( \mathbf{x} \in \mathcal{A} \) and the microscopic (fast) variable \( \xi = \mathbf{x}/\varepsilon \in \mathcal{Q} \) (see for example Bakhvalov and Panasenko (1984); Smyshlyaev (2009) 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: \( C^{(m, \varepsilon)}(\mathbf{x}) = C^m(\xi = \mathbf{x}/\varepsilon), \ K^{(m, \varepsilon)}(\mathbf{x}) = K^m(\xi = \mathbf{x}/\varepsilon) \).
x/\varepsilon), \, \alpha^{(m,e)}(x) = \alpha^m(\xi = x/\varepsilon), D^{(m,e)}(x) = D^m(\xi = x/\varepsilon), \, \beta^{(m,e)}(x) = \beta^m(\xi = x/\varepsilon), \text{ respectively.}

The relevant micro-fields are the micro-displacement \( u(x) \), the microscopic temperature \( \theta(x) = T(x) - T_0 \) and the microscopic mass concentration \( \eta(x) = C(x) - C_0 \) evaluated with respect to the natural state \((T = T_0, C = C_0)\). The micro-stress \( \sigma(x) \), the microscopic heat and mass fluxes \( q(x) \) and \( j(x) \) are defined by the following constitutive relations:

\[
\sigma(x) = C^m \left( \frac{x}{\varepsilon} \right) \varepsilon(x) - \alpha^m \left( \frac{x}{\varepsilon} \right) \theta(x) - \beta^m \left( \frac{x}{\varepsilon} \right) \eta(x),
\]

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

where \( \varepsilon(x) = \text{sym}\nabla u(x) \) is the micro-strain tensor which is assumed to be zero at the fundamental state of the system. The micro-stresses \( \mathbb{1} \) and the microscopic fluxes \( \mathbb{2} \) satisfy the local balance equations on the domain \( \mathcal{A} \)

\[
\nabla \cdot \sigma(x) + b(x) = 0,
\]

\[
\nabla \cdot q(x) - r(x) = 0,
\]

\[
\nabla \cdot j(x) - s(x) = 0.
\]

Substituting expressions \( \mathbb{1} \)-\( \mathbb{5} \) in equations \( \mathbb{6} \)-\( \mathbb{8} \) and remembering the symmetry of the elasticity tensor, the resulting set of partial differential equations is written in the form

\[
\nabla \cdot \left( C^m \left( \frac{x}{\varepsilon} \right) \nabla u(x) \right) - \nabla \cdot \left( \alpha^m \left( \frac{x}{\varepsilon} \right) \theta(x) \right) - \nabla \cdot \left( \beta^m \left( \frac{x}{\varepsilon} \right) \eta(x) \right) + b(x) = 0
\]

\[
\nabla \cdot \left( K^m \left( \frac{x}{\varepsilon} \right) \nabla \theta(x) \right) + r(x) = 0,
\]

\[
\nabla \cdot \left( D^m \left( \frac{x}{\varepsilon} \right) \nabla \eta(x) \right) + s(x) = 0.
\]

The micro-displacement, microscopic temperature and mass concentration may be seen in the form

\( u(x, \xi = x/\varepsilon), \theta(x, \xi = x/\varepsilon), \eta(x, \xi = x/\varepsilon) \) as functions of both the slow and the fast variable. The solution of microscopic fields equations \( \mathbb{9} \), \( \mathbb{10} \) and \( \mathbb{11} \) 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 \( \varepsilon \) 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. \( \mathbb{4} \) 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 \( \varepsilon \) that keeps the dependence on the slow variable \( x \) separate from the fast one \( \xi = x/\varepsilon \) such that two distinct scales are represented.

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

3  Multiscale analysis and asymptotic solution of the heterogeneous problem

Following the approaches developed in Bakhtiyarov and Panasenko (1984), Semyshlyaev and Cherednichenko (2000), Bacigalupo and Gambarotta (2014) and Bacigalupo (2014) for purely elastic problems in periodic heterogeneous media, the microscopic displacement, temperature and mass concentration fields are represented through an asymptotic expansion with respect to the parameter \( \varepsilon \), whose terms depend on macroscopic fields and perturbation functions:

\[
\begin{align*}
u_k \left( x, \xi = \frac{x}{\varepsilon} \right) &= U_k(x) + \sum_{l=1}^{+\infty} \varepsilon^l \sum_{|q|=l} N_{kpq}^{(l)}(\xi) \frac{\partial^l U_p(x)}{\partial x_q} + \\
&+ \sum_{l=1}^{+\infty} \varepsilon^l \sum_{|q|=l} \left( \tilde{N}_{kpq}^{(l)}(\xi) \frac{\partial^l \Theta(x)}{\partial x_q} + \tilde{\Sigma}_{kpq}^{(l)}(\xi) \frac{\partial^{l-1} \Theta(x)}{\partial x_q} \right) \bigg|_{\xi = x/\varepsilon} \\
&= U_k(x) + \varepsilon \left( N_{kpq}^{(1)}(\xi) \frac{\partial U_p(x)}{\partial x_q} + \tilde{N}_{kpq}^{(1)}(\xi) \Theta(x) + \tilde{\Sigma}_{kpq}^{(1)}(\xi) \Theta(x) \right) + \\
&+ \varepsilon^2 \left( N_{kpq1q2}^{(2)}(\xi) \frac{\partial^2 U_p(x)}{\partial x_{q1} \partial x_{q2}} + \tilde{N}_{kpq1}^{(2)}(\xi) \frac{\partial \Theta(x)}{\partial x_{q1}} + \tilde{\Sigma}_{kpq1}^{(2)}(\xi) \frac{\partial \Theta(x)}{\partial x_{q1}} \right) \bigg|_{\xi = x/\varepsilon} + \cdots,
\end{align*}
\]

\[
\begin{align*}
\theta \left( x, \xi = \frac{x}{\varepsilon} \right) &= \Theta(x) + \sum_{l=1}^{+\infty} \varepsilon^l \sum_{|q|=l} \left( M_q^{(l)}(\xi) \frac{\partial \Theta(x)}{\partial x_q} \right) \bigg|_{\xi = x/\varepsilon} \\
&= \Theta(x) + \varepsilon \left( M_{q1}^{(1)}(\xi) \frac{\partial \Theta(x)}{\partial x_{q1}} \right) + \varepsilon^2 \left( M_{q1q2}^{(2)}(\xi) \frac{\partial^2 \Theta(x)}{\partial x_{q1} \partial x_{q2}} \right) \bigg|_{\xi = x/\varepsilon} + \cdots,
\end{align*}
\]

\[
\begin{align*}
\eta \left( x, \xi = \frac{x}{\varepsilon} \right) &= \Upsilon(x) + \sum_{l=1}^{+\infty} \varepsilon^l \sum_{|q|=l} \left( W_q^{(l)}(\xi) \frac{\partial \Upsilon(x)}{\partial x_q} \right) \bigg|_{\xi = x/\varepsilon} \\
&= \Upsilon(x) + \varepsilon \left( W_{q1}^{(1)}(\xi) \frac{\partial \Upsilon(x)}{\partial x_{q1}} \right) + \varepsilon^2 \left( W_{q1q2}^{(2)}(\xi) \frac{\partial^2 \Upsilon(x)}{\partial x_{q1} \partial x_{q2}} \right) \bigg|_{\xi = x/\varepsilon} + \cdots.
\end{align*}
\]
In equations (12), (13) and (14) (commonly known as down-scaling relations), \( q = q_1, \ldots, q_l \) is a multi-index and \( \partial T/\partial x_q = \partial T/\partial x_{q_1} \cdots \partial x_{q_l} \). Due to their dependence on the slow space variable \( x \), the macroscopic fields \( U_k, \Theta \) and \( \Upsilon \) are \( \mathcal{L} \)-periodic functions. \( N_{kpq}^{(l)}, M_q^{(l)} \) and \( W_l^{(l)} \) are the mechanical, thermal and diffusive fluctuations functions, respectively, whereas \( \tilde{N}_{kpq}^{(l)} \) and \( \tilde{N}_{kq}^{(l)} \) denote the additional fluctuations functions corresponding to the contribution of the thermodiffusion to local displacement. All these perturbation functions depend on the fast space variable \( \xi = x/\varepsilon \), and moreover, as it will be shown in Section 3.1, they are \( \mathcal{Q} \)-periodic. Similarly to the procedure reported in Smyshlyaev and Cherednichenko (2000) and Bacigalupo (2014), the mean value of the fluctuations functions is assumed to vanish on the unit cell \( Q \), this means that the following normalization conditions are satisfied:

\[
\langle N_{kpq}^{(l)} \rangle = \frac{1}{\delta} \int_Q N_{kpq}^{(l)}(\xi) d\xi = 0, \quad \langle \tilde{N}_{kpq}^{(l)} \rangle = \frac{1}{\delta} \int_Q \tilde{N}_{kpq}^{(l)}(\xi) d\xi = 0, \quad \langle \tilde{N}_{kq}^{(l)} \rangle = \frac{1}{\delta} \int_Q \tilde{N}_{kq}^{(l)}(\xi) d\xi = 0, \\
\langle M_q^{(l)} \rangle = \frac{1}{\delta} \int_Q M_q^{(l)}(\xi) d\xi = 0, \quad \langle W_l^{(l)} \rangle = \frac{1}{\delta} \int_Q W_l^{(l)}(\xi) d\xi = 0.
\]

(15)

Defining the new variable \( \zeta \in Q \) and the vector \( \epsilon \zeta \in A \), which represents the translations of the media with respect to the \( \mathcal{L} \)-periodic body forces \( b(x) \), heat sources \( r(x) \) and mass sources \( s(x) \) [Bacigalupo and Gambarotta, 2014], for any \( \mathcal{Q} \)-periodic function \( g(\xi + \zeta) \) the following property is verified:

\[
\langle g(\xi + \zeta) \rangle = \frac{1}{\delta} \int_Q g(\xi + \zeta) d\zeta = \frac{1}{\delta} \int_Q g(\xi + \zeta) d\xi.
\]

(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 \( Q \):

\[
U_k(x) \doteq \langle u_k \left(x, \frac{x}{\varepsilon} + \zeta\right) \rangle, \quad \Theta(x) \doteq \langle \theta \left(x, \frac{x}{\varepsilon} + \zeta\right) \rangle, \quad \Upsilon(x) \doteq \langle \eta \left(x, \frac{x}{\varepsilon} + \zeta\right) \rangle.
\]

(17)

Expressions (17) are commonly known as up-scaling relations.

3.1 Asymptotic analysis and derivation of the cell problems

In order to derive exact expressions for the fluctuations functions affecting the behavior of the microscopic fields \( u_k, \theta, \eta \), the down-scaling relations (12), (13) and (14) are substituted into the microscopic fields equations (9), (10) and (11). Remembering the property \( \frac{\partial}{\partial x_j} f(x, \xi = \frac{x}{\varepsilon}) = \)
(\frac{\partial f}{\partial x_j} + \frac{1}{\varepsilon} \frac{\partial f}{\partial \xi_j})_{\xi=\pm\varepsilon} = \left(\frac{\partial f}{\partial x_j} + \frac{f_j}{\varepsilon}\right)_{\xi=\pm\varepsilon}$, equation (1) become

$$
\varepsilon^{-1}\left\{\left[C_{ijkl}(1)_{kpqj,i}\right]_{j} + C_{ijkl}(1)_{j}N_{kpqj,i}\right\}H_{pqj}(x) + \left[C_{ijkl}(1)_{j} - \alpha_{ijkl}\right]\Theta(x)
$$

$$
+ \left[C_{ijkl}(1)_{j} - \beta_{ijkl}\right]Y(x) \right\}
$$

$$
+ \varepsilon^{0}\left\{\left[C_{ijkl}(2)_{j}\right]_{j} + \frac{1}{2}\left[C_{ijkl}(2)_{j}N_{kpqj,i}\right]_{j} + C_{ijkl}(2)_{j}N_{kpqj,i} + C_{ijkl}(2)_{j}N_{kpqj,i}
$$

$$
+ \left[C_{ijkl}(2)_{j} - \alpha_{ijkl}\right]\Theta(x)
$$

$$
+ \left[C_{ijkl}(2)_{j} - \beta_{ijkl}\right]Y(x) \right\}
$$

$$
+ \ldots + b_{i}(x) = 0, \quad i = 1, 2,
$$

(18)

where $H_{pqj} = \partial U_{p}/\partial x_{qj}$ are the components of the macroscopic displacement gradient tensor previously defined, and $\kappa_{pqj2}$ are the elements of the macroscopic second gradient tensor. Equations (10) and (11) assume the following form

$$
\varepsilon^{-1}\left[\left(K_{ij}^{(1)}M_{1qj,i}\right)_{j} + K_{ijq,i}\right]\frac{\partial \Theta}{\partial x_{qj}}
$$

$$
+ \varepsilon^{0}\left[\left(K_{ij}^{(2)}M_{1qj,i}\right)_{j} + \frac{1}{2}\left[K_{ij}^{(2)}M_{1qj,i}\right]_{j} + K_{ijq}^{(2)}M_{1qj,i}\right]\frac{\partial \Theta}{\partial x_{qj}}
$$

$$
+ \ldots + r(x) = 0.
$$

(19)

$$
\varepsilon^{-1}\left[\left(D_{ijk}^{(1)}W_{1qj,i}\right)_{j} + D_{ijkq,i}\right]\frac{\partial Y}{\partial x_{qj}}
$$

$$
+ \varepsilon^{0}\left[\left(D_{ijk}^{(2)}W_{1qj,i}\right)_{j} + \frac{1}{2}\left[D_{ijk}^{(2)}W_{1qj,i}\right]_{j} + D_{qijq}^{(2)}W_{1qj,i}\right]\frac{\partial Y}{\partial x_{qj}}
$$

$$
+ \ldots + s(x) = 0.
$$

(20)

In order to transform the fields equation (18), (19) and (20) in a PDEs system with constant coefficients, in which the unknowns are the macroscopic quantities $U_{k}(x)$, $\Theta(x)$ and $Y(x)$, the fluctuations functions have to satisfy non-homogeneous equations (cell problems) reported below.
At the order \( \varepsilon^{-1} \) from the equation \((\ref{eq:18})\) we derive:

\[
\begin{align*}
\left( C_{ijkl} N_{kpq1,l}^{(1)} \right)_{ij} + C_{ijpq1,i}^{(1)} = n_{ipq1}^{(1)}, \\
\left( C_{ijkl} N_{k,l}^{(1)} \right)_{ij} - \alpha_{ij,l}^{(1)} = \tilde{n}_{i}^{(1)}, \\
\left( C_{ijkl} \tilde{N}_{k,l}^{(1)} \right)_{ij} - \beta_{ij,l}^{(1)} = \check{n}_{i}^{(1)},
\end{align*}
\]

(21)

whereas from thermodiffusion equations \((\ref{eq:19})\) and \((\ref{eq:20})\) we obtain:

\[
\begin{align*}
\left( K_{ij} M_{q1,i}^{(1)} \right)_{ij} + K_{iq1}^{(1)} = m_{q1}^{(1)}, \\
\left( D_{ij} W_{q1,i}^{(1)} \right)_{ij} + D_{iq1}^{(1)} = w_{q1}^{(1)},
\end{align*}
\]

(22)

where:

\[
\begin{align*}
n_{ipq1}^{(1)} &= \left( C_{ijkl} N_{k,pq1}^{(2)} \right)_{i} = 0, \\
\tilde{n}_{i}^{(1)} &= -\left( \alpha_{ij,l}^{(1)} \right) = 0, \\
\check{n}_{i}^{(1)} &= -\left( \beta_{ij,l}^{(1)} \right) = 0, \\
m_{q1}^{(1)} &= \left( K_{ij} M_{q1}^{(1)} \right)_{ij} = 0, \\
w_{q1}^{(1)} &= \left( D_{ij} W_{q1}^{(1)} \right)_{ij} = 0.
\end{align*}
\]

(23)

The properties \((\ref{eq:26})\) are consequence of the \(Q\)-periodicity of the components \(C_{ijkl}, \alpha_{ij,l}^{(1)}, \beta_{ij,l}^{(1)}, K_{iq1}^{(1)}\), and \(D_{iq1}^{(1)}\). At the order \( \varepsilon^0 \), equation \((\ref{eq:18})\) yield

\[
\begin{align*}
\left( C_{ijkl} N_{k,pq1}^{(2)} \right)_{i} + \frac{1}{2} \left( C_{ijkl} N_{k,pq2}^{(2)} \right)_{i} + C_{ijkl} N_{k,pq2}^{(1)} + C_{ijkl} N_{k,pq1}^{(1)} + C_{ijkl} N_{k,pq2}^{(1)} - \alpha_{ij,l}^{(1)} - \left( \alpha_{ij} M_{q1}^{(1)} \right)_{ij} = n_{ipq1}^{(2)}, \\
\left( C_{ijkl} \tilde{N}_{k,l}^{(2)} \right)_{i} + \left( C_{ijkl} \tilde{N}_{k,l}^{(2)} \right)_{i} + C_{ijkl} \tilde{N}_{k,l}^{(1)} - \alpha_{ij,l}^{(1)} - \left( \alpha_{ij} M_{q1}^{(1)} \right)_{ij} = \tilde{n}_{i}^{(2)}, \\
\left( C_{ijkl} \check{N}_{k,l}^{(2)} \right)_{i} + \left( C_{ijkl} \check{N}_{k,l}^{(2)} \right)_{i} + C_{ijkl} \check{N}_{k,l}^{(1)} - \beta_{ij,l}^{(1)} - \left( \beta_{ij} W_{q1}^{(1)} \right)_{ij} = \check{n}_{i}^{(2)},
\end{align*}
\]

(24)

at the same order, from \((\ref{eq:19})\) and \((\ref{eq:20})\) we derive:

\[
\begin{align*}
\left( K_{ij} M_{q1,q2}^{(2)} \right)_{ij} + \frac{1}{2} \left( K_{ij} M_{q1,q2}^{(2)} \right)_{ij} + K_{q2} M_{q1}^{(1)} + K_{q1} M_{q2}^{(1)} &= m_{q1,q2}^{(2)}, \\
\left( D_{ij} W_{q1,q2}^{(2)} \right)_{ij} + \frac{1}{2} \left( D_{ij} W_{q1,q2}^{(2)} \right)_{ij} + D_{q1} W_{q2}^{(1)} + D_{q2} W_{q1}^{(1)} &= w_{q1,q2}^{(2)}
\end{align*}
\]

(25) (26)

where:

\[
\begin{align*}
n_{ipq1,q2}^{(2)} &= \frac{1}{2} \left( C_{ijkl} N_{k,pq1}^{(1)} + C_{ijkl} N_{k,pq2}^{(1)} + C_{ijkl} N_{k,pq1}^{(1)} + C_{ijkl} N_{k,pq2}^{(1)} \right),
\end{align*}
\]

9
whereas the thermodiffusive cell problems corresponding to equations (19) and (20) are:

\[ \dot{n}_{iq1}^{(2)} = \left\langle C_{i}^{\epsilon}_{iq1} k_{i} \dot{N}_{1,kl}^{(1)} - \alpha_{i}^{\epsilon} n_{iq1} \right\rangle, \quad \dot{n}_{iq1}^{(2)} = \left\langle C_{i}^{\epsilon}_{iq1} k_{i} \dot{N}_{1,kl}^{(1)} - \beta_{i}^{\epsilon} n_{iq1} \right\rangle, \]

\[ m_{iq1,q2}^{(2)} = \frac{1}{2} \left\langle K_{q2,q1}^{\epsilon} + K_{q1,q2}^{\epsilon} M_{q1,q2}^{(1)} + K_{q2,q1}^{\epsilon} M_{q1,q2}^{(1)} \right\rangle, \]

\[ w_{iq1,q2}^{(2)} = \frac{1}{2} \left\langle D_{q2,q1}^{\epsilon} + D_{q1,q2}^{\epsilon} W_{q1,q2}^{(1)} + D_{q2,q1}^{\epsilon} W_{q1,q2}^{(1)} \right\rangle. \]

(27)

For the \( m - 2 \) order, the cells problems associate to equation (18) assume the general form:

\[ \left( C_{ijkl} N_{q1}^{(m)} \right)_{i,j}^{(2)} + \frac{1}{m!} \sum_{q(q)} \left[ \left( C_{ijkl}^{\epsilon} N_{q1}^{(m-1)} \right)_{i,j} + C_{ijkl}^{\epsilon} N_{q1}^{(m-2)} \right] = \hat{n}_{iq1}^{(m)}, \]

\[ \left( C_{ijkl}^{\epsilon} N_{q1}^{(m)} \right)_{i,j}^{(2)} + \frac{1}{m!} \sum_{q(q)} \left[ \left( C_{ijkl}^{\epsilon} N_{q1}^{(m-1)} \right)_{i,j} + C_{ijkl}^{\epsilon} N_{q1}^{(m-2)} \right] = \hat{n}_{iq1}^{(m-1)} \]

\[ \left( C_{ijkl}^{\epsilon} N_{q1}^{(m)} \right)_{i,j}^{(2)} + \frac{1}{m!} \sum_{q(q)} \left[ \left( C_{ijkl}^{\epsilon} N_{q1}^{(m-1)} \right)_{i,j} + C_{ijkl}^{\epsilon} N_{q1}^{(m-2)} \right] = \hat{n}_{iq1}^{(m-2)}, \]

(28)

whereas the thermodiffusive cell problems corresponding to equations (19) and (20) are:

\[ \left( K_{ijkl}^{\epsilon} M_{q1}^{(m)} \right)_{i,j} \]

\[ \left( C_{ijkl}^{\epsilon} N_{q1}^{(m-1)} \right)_{i,j}^{(2)} + \frac{1}{m!} \sum_{q(q)} \left[ \left( C_{ijkl}^{\epsilon} N_{q1}^{(m-1)} \right)_{i,j} + C_{ijkl}^{\epsilon} N_{q1}^{(m-2)} \right] = m_{q1}^{(m)}, \]

(29)

\[ \left( D_{ijkl}^{\epsilon} W_{q1}^{(m)} \right)_{i,j}^{(2)} \]

\[ \left( D_{ijkl}^{\epsilon} W_{q1}^{(m-1)} \right)_{i,j}^{(2)} + \frac{1}{m!} \sum_{q(q)} \left[ \left( D_{ijkl}^{\epsilon} W_{q1}^{(m-1)} \right)_{i,j} + D_{ijkl}^{\epsilon} W_{q1}^{(m-2)} \right] = w_{q1}^{(m)}, \]

(30)

where the symbol \( p(q) \) denotes all possible permutations of the multi-index \( q \), and the constants \( n_{iq1,q2}, n_{iq1,q2}, n_{iq1,q2}, n_{iq1,q2}, n_{iq1,q2}, n_{iq1,q2} \) are defined as follows:

\[ n_{iq1,q2}^{(m)} = \frac{1}{m!} \sum_{p(q)} \left\langle C_{ijkl}^{\epsilon} N_{pq1}^{(m)} \right\rangle, \]

\[ n_{iq1,q2}^{(m)} = \frac{1}{m!} \sum_{p(q)} \left\langle C_{ijkl}^{\epsilon} N_{pq1}^{(m)} \right\rangle, \]

\[ n_{iq1,q2}^{(m)} = \frac{1}{m!} \sum_{p(q)} \left\langle C_{ijkl}^{\epsilon} N_{pq1}^{(m)} \right\rangle, \]
\[
\begin{align*}
\hat{n}^{(m)}_{iq_1\ldots q_{m-1}} &= \frac{1}{m!} \sum_{P(q)} \left\langle C^{\varepsilon}_{q_{m-1}kq_{m-2}} \hat{N}^{(m-2)}_{q_{k}\ldots q_{m-3}} + C^{\varepsilon}_{q_{m-1}kl} \hat{N}^{(m-1)}_{q_{l}\ldots q_{m-2}}l - \beta^{\varepsilon} u_{q_{m-1}} W^{(m-2)}_{q_1\ldots q_{m-2}} \right\rangle, \\
m^{(m)}_{q_{1}\ldots q_{m}} &= \frac{1}{m!} \sum_{P(q)} \left\langle K^{\varepsilon}_{q_{m}q_{1}} M^{(m-2)}_{q_{2}\ldots q_{m-1}} + K^{\varepsilon}_{q_{m}j} M^{(m-1)}_{q_{1}\ldots q_{m-1}j} \right\rangle, \\
w^{(m)}_{q_{1}\ldots q_{m}} &= \frac{1}{m!} \sum_{P(q)} \left\langle D^{\varepsilon}_{q_{m}q_{1}} W^{(m-2)}_{q_{2}\ldots q_{m-1}} + D^{\varepsilon}_{q_{m}j} W^{(m-1)}_{q_{1}\ldots q_{m-1}j} \right\rangle. (31)
\end{align*}
\]

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 (20), (27) and (31) are determined by imposing that the non-homogeneous terms in equations (21), (22), (25), (24), (26), (29) and (30) (associated to the auxiliary body forces (Bacigalupo, 2014), heat and mass sources) possess vanishing mean values over the unit cell \( Q \). This implies the \( Q \)-periodicity of the perturbations functions \( N^{(m)}_{kpq}, \tilde{N}^{(m)}_{kq_{1}}, \hat{N}^{(m)}_{q_{k}}, M^{(m)}_{q_{1}\ldots q_{m-1}}, W^{(m)}_{q} \), 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. Using the cell problems (21), (22), (24), (25), (26), (29) and (30) together with the constants definitions (20), (24) and (31) into the microscopic fields equations (13), (19) and (20), the averaged equations of infinite order are derived:

\[
\begin{align*}
n^{(2)}_{ipq_{1}q_{2}} \frac{\partial^2 U_p}{\partial x_{q_1} \partial x_{q_2}} + n^{(2)}_{iq_1} \frac{\partial \Theta}{\partial x_{q_1}} + n^{(2)}_{iq_1} \frac{\partial \Upsilon}{\partial x_{q_1}} + \sum_{n=0}^{+\infty} \varepsilon^{n+1} \sum_{|q|=n+3} \hat{n}^{(n+3)}_{ipq} \frac{\partial^{n+3} U_p}{\partial x_{q}} = 0, \\
m^{(2)}_{q_{1}q_{2}} \frac{\partial^2 \Theta}{\partial x_{q_1} \partial x_{q_2}} + \sum_{n=0}^{+\infty} \varepsilon^{n+1} \sum_{|q|=n+3} m^{(n+3)}_{q} \frac{\partial^{n+3} \Theta}{\partial x_{q}} = 0, \\
w^{(2)}_{q_{1}q_{2}} \frac{\partial^2 \Upsilon}{\partial x_{q_1} \partial x_{q_2}} + \sum_{n=0}^{+\infty} \varepsilon^{n+1} \sum_{|q|=n+3} w^{(n+3)}_{q} \frac{\partial^{n+3} \Upsilon}{\partial x_{q}} = 0,
\end{align*}
\]

where \( q \) is a multi-index, \( \partial^{n+1} (\cdot)/\partial x_{q} = \partial^{n+2} (\cdot)/\partial x_{q_1} \cdots \partial x_{q_{n+1}} \) with \( j \in \mathbb{N}, n^{(n+3)}_{ipq_{1}q_{2} \ldots q_{n+2}} = n^{(n+3)}_{ipq_{1} \ldots q_{n+2}}, n^{(n+2)}_{q_{1}q_{2}q_{3}} = n^{(n+2)}_{i_{q_{1}} \ldots q_{n+2}}, m^{(n+3)}_{q_{1}q_{2}q_{3} \ldots q_{n+2}} = m^{(n+3)}_{q_{1} \ldots q_{n+2}} \) and \( w^{(n+3)}_{q_{1}q_{2}q_{3} \ldots q_{n+2}} = w^{(n+3)}_{q_{1} \ldots q_{n+2}} \).

### 3.2 Formal solution of averaged fields equation of infinite order

A formal solution of the averaged field equations of infinite order (22), (26) and (31) is obtained by means of an asymptotic expansion of the macroscopic fields \( U_i, \Theta \) and \( \Upsilon \) in terms of the microstructural size \( \varepsilon \), i.e.

\[
\begin{align*}
U_i(x) &= \sum_{j=0}^{+\infty} \varepsilon^m U^{(m)}_i(x), \quad \Theta(x) = \sum_{j=0}^{+\infty} \varepsilon^m \Theta^{(m)}(x), \quad \Upsilon(x) = \sum_{j=0}^{+\infty} \varepsilon^m \Upsilon^{(m)}(x).
\end{align*}
\]
By substituting the series \( \hat{U}_p^{(0)} \), \( \hat{\Theta}_q^{(0)} \) and \( \hat{\Upsilon}_r^{(0)} \), 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 \( \epsilon^0 \), from the equation (32) we derive:

\[
\begin{align*}
\hat{n}^{(2)}_{ipq_1, q_2} \frac{\partial^2 U_p^{(0)}}{\partial x_{q_1} \partial x_{q_2}} + \hat{n}^{(2)}_{i q_1} \frac{\partial \Theta^{(0)}}{\partial x_{q_1}} + \hat{n}^{(2)}_{i q_1} \frac{\partial \Upsilon^{(0)}}{\partial x_{q_1}} + b_i = 0,
\end{align*}
\]

(36)

whereas thermodiffusion equations (33) and (34) yield respectively

\[
\begin{align*}
\hat{m}^{(2)}_{q_1, q_2} \frac{\partial^2 \Theta^{(0)}}{\partial x_{q_1} \partial x_{q_2}} + r = 0,
\end{align*}
\]

(37)

\[
\begin{align*}
\hat{w}^{(2)}_{q_1, q_2} \frac{\partial^2 \Upsilon^{(0)}}{\partial x_{q_1} \partial x_{q_2}} + s = 0.
\end{align*}
\]

(38)

At the generic order \( m \) from (32) we obtain

\[
\begin{align*}
\hat{n}^{(2)}_{ipq_1, q_2} \frac{\partial^2 U_p^{(m)}}{\partial x_{q_1} \partial x_{q_2}} + \hat{n}^{(2)}_{i q_1} \frac{\partial \Theta^{(m)}}{\partial x_{q_1}} + \hat{n}^{(2)}_{i q_1} \frac{\partial \Upsilon^{(m)}}{\partial x_{q_1}} + \sum_{r=3}^{m+2} \sum_{|q|=r-1} \hat{n}^{(r)}_{iq} \frac{\partial^{r-1} U_p^{(m+2-r)}}{\partial x_{q_1} \partial x_{q_2}} = 0,
\end{align*}
\]

(39)

and (33) and (34) are given by

\[
\begin{align*}
\hat{m}^{(2)}_{q_1, q_2} \frac{\partial^2 \Theta^{(m)}}{\partial x_{q_1} \partial x_{q_2}} + \sum_{p=3}^{m+2} \sum_{|h|=p} m^{(p)}_{h} \frac{\partial \Theta^{(m+2-p)}}{\partial x_{h}} = 0,
\end{align*}
\]

(40)

\[
\begin{align*}
\hat{w}^{(2)}_{q_1, q_2} \frac{\partial^2 \Upsilon^{(m)}}{\partial x_{q_1} \partial x_{q_2}} + \sum_{p=3}^{m+2} \sum_{|h|=p} w^{(p)}_{h} \frac{\partial \Upsilon^{(m+2-p)}}{\partial x_{h}} = 0,
\end{align*}
\]

(41)

where \( h \) and \( q \) are multi-indexes. The solution of equations (36)-(41) requires that the following normalization condition is satisfied:

\[
\begin{align*}
\frac{1}{\delta L^2} \int_L U_p^{(m)}(x) dx = 0, \quad \frac{1}{\delta L^2} \int_L \Theta^{(m)}(x) dx = 0, \quad \frac{1}{\delta L^2} \int_L \Upsilon^{(m)}(x) dx = 0,
\end{align*}
\]

(42)

where the \( L \)–periodic domain is the same defined in previous Section as \( L = [0, L] \times [0, \delta L] \).

The averaged field equation \( \text{(32), (33) and (34)} \) (or alternatively the sequence of PDEs \( \text{(36)-(41)} \)), obtained by means of the proposed rigorous asymptotic procedure, are now used for deriving the fields equation of the first order (Cauchy) homogeneous continuum equivalent to the considered periodic thermodiffusive material. As it will be demonstrated in the next Section, the fields equation of the first order homogeneous continuum can be obtained by the zero order terms (equations (36), (37) and (38)) of the sequence of PDEs derived applying the asymptotic analysis to the averaged field equation. This implies that the macroscopic displacement, temperature and mass concentration are approximated as follows:

\[
\begin{align*}
U_p(x) \approx U_p^{(0)}(x), \quad \Theta(x) \approx \Theta^{(0)}(x), \quad \Upsilon(x) \approx \Upsilon^{(0)}(x).
\end{align*}
\]

(43)
Alternatively, the field equation of the equivalent Cauchy continuum can be derived considering only the terms of order \( \varepsilon^0 \) in the equations (32), (33) and (34).

The approximation of the average field equations (32)-(34) yielded by solution of homogenized differential problems of generic order \( m \) is more accurate with respect to that obtained by the assumption (33). This implies also a more precise approximation of the solution of the microscopic field equation (9)-(11) by means of the down-scaling relation (13), (19) and (20) involving the macroscopic field (35). 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 (32)-(34) at a generic order \( m \) has 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.

4 Homogenized thermodiffusive Cauchy continuum: field equations and overall properties

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

\[
C_{iq_1pq_2} \frac{\partial^2 U_p}{\partial x_{q_1} \partial x_{q_2}} - \alpha_{iq_1} \frac{\partial \Theta}{\partial x_{q_1}} - \beta_{iq_1} \frac{\partial \Upsilon}{\partial x_{q_1}} + b_i = 0,
\]

\[
K_{iq_2} \frac{\partial^2 \Theta}{\partial x_{q_2} \partial x_{q_2}} + r = 0,
\]

\[
D_{iq_2} \frac{\partial^2 \Upsilon}{\partial x_{q_2} \partial x_{q_2}} + s = 0,
\]

where \( C_{iq_1pq_2} \) are the components of the overall elastic tensor, \( \alpha_{iq_1} \) and \( \beta_{iq_1} \) are respectively the components of the overall thermal dilatation and diffusive expansion tensors, \( K_{iq_2} \) denotes the components of the overall heat conduction tensor and \( D_{iq_2} \) represents the components of the overall mass diffusion tensor. Remembering the approximation (43), the macroscopic field equations (44), (45) and (46) can be compared to the zero order terms of the averaged field equation (36), (37) and (38) for determining the overall properties of the thermodiffusive Cauchy continuum. In order to relate the coefficients \( n_{ipq_1q_2}, \hat{n}_{iq_1}, \hat{\alpha}_{iq_1}, m_{iq_1q_2}, w_{iq_1q_2} \) contained in the equations (36), (37) and (38) to the overall elastic and thermodiffusive constants of the media \( C_{iq_1pq_2}, \alpha_{iq_1}, \beta_{iq_1}, K_{iq_1q_2}, D_{iq_1q_2} \), the symmetries of the tensors of components \( n_{ipq_1q_2}, \hat{n}_{iq_1}, \hat{\alpha}_{iq_1}, m_{iq_1q_2}, w_{iq_1q_2} \), and the ellipticity of the fields equations (36), (37), and (38) are required. A demonstration of these properties is reported in Appendix A. As a consequence of these properties, it can be observed that: \( n_{ipq_1q_2} = \frac{1}{2}(C_{iq_1pq_2} + C_{iq_2pq_1}), \hat{n}_{iq_1} = \alpha_{iq_1}, \hat{\alpha}_{iq_1} = \beta_{iq_1}, m_{iq_1q_2} = K_{iq_1q_2} \) and \( w_{iq_1q_2} = D_{iq_1q_2} \). In particular, comparing the field equation (44) to (36), and remembering the relationship between \( n_{ipq_1q_2} \) and...
\[ C_{q_1q_2} \text{, it is easy to note that due to the repetition of the indexes } q_1 \text{ and } q_2: \]
\[ C_{q_1q_2} \frac{\partial^2 U_p}{\partial x_{q_1} \partial x_{q_2}} = n_{q_1q_2} \frac{\partial^2 U_p}{\partial x_{q_1} \partial x_{q_2}}. \]

The overall elastic and thermodynamic tensors, obtained in terms of fluctuations functions, and the components of microscopic elastic and thermodynamic tensors, take the form (see Appendix A for details):
\[
C_{q_1q_2} = \frac{1}{4} \left( \delta_{q_1q_2} + \delta_{q_2q_1} \right) \left( \delta_{q_1q_2} + \delta_{q_2q_1} \right).
\]

The components \( C_{q_1q_2} \) 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 Cherndichenko, 2000; Bacigalupo, 2014) and heat conduction problems (Zhang et al., 2007) in media with periodic microstructures. The components \( \alpha_{q_1} \) and \( \beta_{q_1} \) of the coupling thermodynamic 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, mass concentration 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 thermodynamic constants are derived. Considering a two-dimensional infinite thermodynamic 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.

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 \( e_1 \), the geometry of the system is shown in Fig. 2. The orthotropic symmetry is assumed
functions \( N_{riq}^{(1)} \), \( \tilde{N}_{k}^{(1)} \), \( \hat{N}_{k}^{(1)} \), \( M_{q}^{(1)} \) and \( W_{q}^{(1)} \) are analytically obtained through the solution of the cell problems formulated in Section 3.1 (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 \( \xi_2 \). This variable is perpendicular to the layering direction \( \epsilon_1 \) (see Fig. 2). The non-vanishing micro-fluctuation functions \( N_{riq}^{(1)} \), \( \tilde{N}_{k}^{(1)} \) and \( \hat{N}_{k}^{(1)} \), obtained by solving the cell problem of order \( \epsilon^{-1} \) (21) are:

\[
N_{211}^{(1)} = \frac{C_{1122}^b - C_{1122}^a}{C_{2222}^a - \zeta C_{2222}^b} \xi_2^a, \quad N_{211}^{(1)} = \zeta \frac{C_{1122}^a - C_{1122}^b}{C_{2222}^a - \zeta C_{2222}^b} \xi_2^b;
\]

\[
N_{222}^{(1)} = \frac{C_{2222}^b - C_{2222}^a}{C_{2222}^a - \zeta C_{2222}^b} \xi_2^a, \quad N_{211}^{(1)} = \zeta \frac{C_{1122}^a - C_{1122}^b}{C_{2222}^a - \zeta C_{2222}^b} \xi_2^b;
\]

\[
N_{112}^{(1)} = N_{121}^{(1)} = \frac{C_{1212}^b - C_{1212}^a}{C_{1212}^a - \zeta C_{1212}^b} \xi_2^a; \quad N_{112}^{(1)} = \zeta \frac{C_{1212}^a - C_{1212}^b}{C_{1212}^a - \zeta C_{1212}^b} \xi_2^b;
\]

\[
\tilde{N}_{2}^{(1)} = \frac{\alpha_{22}^b - \alpha_{22}^a}{C_{2222}^a + \zeta C_{2222}^b} \xi_2^a; \quad \tilde{N}_{2}^{(1)} = \zeta \frac{\alpha_{22}^a - \alpha_{22}^b}{C_{2222}^a + \zeta C_{2222}^b} \xi_2^b;
\]

\[
\hat{N}_{2}^{(1)} = \frac{\beta_{22}^b - \beta_{22}^a}{C_{2222}^a + \zeta C_{2222}^b} \xi_2^a; \quad \hat{N}_{2}^{(1)} = \zeta \frac{\beta_{22}^a - \beta_{22}^b}{C_{2222}^a + \zeta C_{2222}^b} \xi_2^b;
\]

where \( \xi_2^a \in \left[ -\frac{1}{2(\epsilon_{1}+1)}, -\frac{1}{2(\epsilon_{1}+1)} \right] \) and \( \xi_2^b \in \left[ -\frac{1}{2(\epsilon_{1}+1)}, -\frac{1}{2(\epsilon_{1}+1)} \right] \) 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 \( \epsilon^{-1} \) (22) are:

\[
M_{2}^{(1)} = \frac{K_{22}^{a} - K_{22}^{b}}{K_{22}^{a} - \zeta K_{22}^{b}} \xi_2^a; \quad M_{2}^{(1)} = \zeta \frac{K_{22}^{a} - K_{22}^{b}}{K_{22}^{a} - \zeta K_{22}^{b}} \xi_2^b;
\]

\[
W_{2}^{(1)} = \frac{D_{22}^{a} - D_{22}^{b}}{D_{22}^{a} - \zeta D_{22}^{b}} \xi_2^a; \quad W_{2}^{(1)} = \zeta \frac{D_{22}^{a} - D_{22}^{b}}{D_{22}^{a} - \zeta D_{22}^{b}} \xi_2^b.
\]

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.
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 fluctuations functions \([18], [19], [50], [51]\) and \([52]\) are used into expressions \([47]\). The components of the overall elastic tensor \( C_{ijkl} \) take the form:

\[
C_{1111} = \frac{\zeta^2 C_{1111}^{ab} + \zeta (C_{1111}^{ab} C_{2222}^{bc} - (C_{1122}^{ab})^2 + 2C_{1122}^{ab} C_{1111}^{abc} + C_{1111}^{abc})}{(\zeta + 1)(C_{2222}^{ab} + \zeta C_{2222}^{bc})};
\]

\[
C_{2222} = \frac{(\zeta + 1) C_{2222}^{ab}}{C_{2222}^{ab} + \zeta C_{2222}^{bc}};
\]

\[
C_{1212} = \frac{(\zeta + 1) C_{1212}^{ab}}{C_{1212}^{ab} + \zeta C_{1212}^{bc}};
\]

\[
C_{1122} = \frac{C_{1122}^{ab} + \zeta C_{1122}^{bc}}{C_{1122}^{ab} + \zeta C_{1122}^{bc}}.
\]

The non-vanishing components of the thermal dilatation tensor \( \alpha_{1q} \) and diffusive expansion tensor \( \beta_{1q} \) are respectively given by

\[
\alpha_{11} = -\frac{\zeta (C_{1122}^{ab} \alpha_{22} - C_{1122}^{ab} \alpha_{11} - C_{2222}^{ab} \alpha_{11} - C_{1111}^{abc} \alpha_{22} + C_{1111}^{abc} \alpha_{22} - C_{2222}^{abc} \alpha_{11}) - \zeta^2 C_{2222}^{abc} \alpha_{11} - C_{2222}^{abc} \alpha_{22}}{(\zeta + 1)(C_{2222}^{ab} + \zeta C_{2222}^{bc})};
\]

\[
\alpha_{22} = \frac{\zeta C_{2222}^{abc} \alpha_{22} + \zeta C_{2222}^{abc} \alpha_{11}}{C_{2222}^{ab} + \zeta C_{2222}^{bc}};
\]

\[
\beta_{11} = -\frac{\zeta (C_{1122}^{ab} \beta_{22} - C_{1122}^{ab} \beta_{12} - C_{2222}^{ab} \beta_{11} - C_{1111}^{abc} \beta_{22} + C_{1111}^{abc} \beta_{22} - C_{2222}^{abc} \beta_{11}) - \zeta^2 C_{2222}^{abc} \beta_{11} - C_{2222}^{abc} \beta_{22}}{(\zeta + 1)(C_{2222}^{ab} + \zeta C_{2222}^{bc})};
\]

\[
\beta_{22} = \frac{\zeta C_{2222}^{abc} \beta_{22} + \zeta C_{2222}^{abc} \beta_{12}}{C_{2222}^{ab} + \zeta C_{2222}^{bc}}.
\]

The non-vanishing components of the heat conduction tensor \( K_{1q} \) and mass diffusion tensor \( D_{1q} \) take the form

\[
K_{11} = \frac{K_{11}^a + \zeta K_{11}^b}{\zeta + 1};
\]

\[
K_{22} = \frac{(\zeta + 1) K_{22}^a K_{22}^b}{K_{22}^a + \zeta K_{22}^b};
\]

\[
D_{11} = \frac{D_{11}^a + \zeta D_{11}^b}{\zeta + 1};
\]

\[
D_{22} = \frac{(\zeta + 1) D_{22}^a D_{22}^b}{D_{22}^a + \zeta D_{22}^b}.
\]

Considering the case of isotropic phases, the components of the elasticity tensor become \( C_{1111} = C_{2222} = \frac{E_\zeta}{1-\nu_\zeta}; \)

\[
C_{1122} = \frac{\nu_\zeta}{1-\nu_\zeta}, \quad C_{1212} = \frac{E_\zeta}{2(1+\nu_\zeta)}, \quad (with \ zeta = a, b), \ where \ for \ plane-strain: \ E_\zeta = \frac{E_\zeta}{1-\nu_\zeta}, \ 
\]

\[
\nu_\zeta = \frac{\nu_\zeta}{1-\nu_\zeta}, \ \text{whereas \ for \ plane-stress:} \ E_\zeta = E_\zeta, \ \nu_\zeta = \nu_\zeta, \ \text{being} \ E_\zeta \ \text{the Young's \ modulus \ and} \ \nu_\zeta. \]
the Poisson’s ratio, respectively. The components of the thermal dilatation and diffusive expansion tensors take respectively the forms: $\alpha_{11}^{\text{a}} = \alpha_{22}^{\text{a}} = \alpha$, $\beta_{11}^{\text{a}} = \beta_{22}^{\text{a}} = \beta$ (note that the coefficients $\alpha$ and $\beta$ 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 $K_{11}^{\text{a}} = K_{22}^{\text{a}} = K^a$ and $D_{11}^{\text{a}} = D_{22}^{\text{a}} = D^a$. The overall elastic and thermodiffusive constants for the case of isotropic phases are reported in Appendix B. An asymptotic expansion of the constants (54), (55), (56), (57) and (58) in the concentration of the two constituents phases is performed in Appendix C. By the asymptotic expressions reported in this Appendix it can be observed that, if the concentration of the phase $a$ vanishes, expressions (52), (53), (54), (55), and (56) tend to the overall elastic and thermodiffusive constants of the 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 B are used. These constants can be represented in the non-dimensional form:

$$
\tilde{C}_{iq1, pq2}(\varrho_C, \zeta, \tilde{v}_a, \tilde{v}_b) = \frac{C_{iq1, pq2}}{C_{i1, pq2}}, \quad \tilde{\alpha}_{iq1}(\varrho_C, \varrho_a, \zeta, \tilde{v}_a, \tilde{v}_b) = \frac{\alpha_{iq1}}{\alpha_{iq1}}, \quad \tilde{\beta}_{iq1}(\varrho_C, \varrho_b, \zeta, \tilde{v}_a, \tilde{v}_b) = \frac{\beta_{iq1}}{\beta_{iq1}},
$$

$$
\tilde{K}_{iq1}(\varrho_K, \zeta) = \frac{K_{iq1}}{K_{i1}}, \quad \tilde{D}_{iq1}(\varrho_D, \zeta) = \frac{D_{iq1}}{D_{i1}},
$$

where $\varrho_C = \tilde{E}_a / \tilde{E}_b$, $\varrho_a = \tilde{\alpha}^a / \tilde{\alpha}^b$, $\varrho_b = \tilde{\beta}^a / \tilde{\beta}^b$, $\varrho_K = K^a / K^b$, $\varrho_D = D^a / D^b$, and $\tilde{C}_{iq1, pq2} = (C_{iq1, pq2}^a + C_{iq1, pq2}^b)/2, \tilde{\alpha}_{iq1} = (\alpha_{iq1}^a + \alpha_{iq1}^b)/2, \tilde{\beta}_{iq1} = (\beta_{iq1}^a + \beta_{iq1}^b)/2, \tilde{K}_{iq1} = (K_{iq1}^a + K_{iq1}^b)/2, \tilde{D}_{iq1} = (D_{iq1}^a + D_{iq1}^b)/2$. 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 (58) possess the following property:

$$
\tilde{C}_{iq1, pq2}(\varrho_C, \zeta, \tilde{v}) = \tilde{C}_{iq1, pq2}(\varrho_C^{-1}, \zeta^{-1}, \tilde{v}), \quad \tilde{\alpha}_{iq1}(\varrho_C, \varrho_a, \zeta, \tilde{v}) = \tilde{\alpha}_{iq1}(\varrho_C^{-1}, \varrho_a^{-1}, \zeta^{-1}, \tilde{v}),
$$

$$
\tilde{\beta}_{iq1}(\varrho_C, \varrho_a, \zeta, \tilde{v}) = \tilde{\beta}_{iq1}(\varrho_C^{-1}, \varrho_a^{-1}, \zeta^{-1}, \tilde{v}), \quad \tilde{K}_{iq1}(\varrho_K, \zeta) = \tilde{K}_{iq1}(\varrho_K^{-1}, \zeta^{-1}), \quad \tilde{D}_{iq1}(\varrho_D, \zeta) = \tilde{D}_{iq1}(\varrho_D^{-1}, \zeta^{-1}).
$$

The variation of the normalized components of the overall elasticity tensor $\tilde{C}_{1111}, \tilde{C}_{2222}, \tilde{C}_{1212}$ and $\tilde{C}_{1122}$ with the ratio $\varrho_C$ is reported in Figs. 3(a), 4(a), 5(a) and 6(a). The same value of the Poisson’s coefficient $\tilde{v} = 0.3$ has been assumed for both the phases, and several values of the non-dimensional geometrical parameter $\zeta$ has been considered for the computations. It can be observed that for $\varrho_C = 1$, corresponding to the case of two isotropic phases having identical elastic properties, the non-dimensional components of the overall elastic tensor assume the value $\tilde{C}_{iq1, pq2} = 1$ (i.e. $C_{iq1, pq2} = C_{iq1, pq2}^a = C_{iq1, pq2}^b$). In Figs. 3(b), 4(b), 5(b) and 6(b) the components $\tilde{C}_{1111}, \tilde{C}_{2222}, \tilde{C}_{1212}$ and $\tilde{C}_{1122}$ are plotted as functions of $\zeta$ for different values of $\varrho_C$ considering the fixed Poisson’s coefficient $\tilde{v} = 0.3$ identical for both the phases. For $\zeta \to 0$, the thickness of the phase $a$ vanishes. Consequently, the values of the overall elastic constants tends to those of the phase $b$: $C_{iq1, pq2} = C_{iq1, pq2}^b$, and the limit values assumed by the normalized components of the elastic tensor reported in the figures are $\tilde{C}_{iq1, pq2} = 2/(1 + \varrho_C)$. Conversely, for $\zeta \to +\infty$ the thickness of the phase $b$ tends to zero, and then $\tilde{C}_{iq1, pq2} = C_{iq1, pq2}^a$ and the non-dimensional constants plotted in Figs. 3(b), 4(b) assume the limit values $\tilde{C}_{iq1, pq2} = 2\varrho_C/(1 + \varrho_C)$.
Figure 3: (a) Dimensionless constant $\hat{C}_{1111}$ vs. the ratio $\rho_C$ for $\tilde{v}_a = \tilde{v}_b = 0.3$ and for different values of the geometric ratio $\zeta$: $\zeta = 1/10$ 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 $\hat{C}_{1111}$ vs. the geometric ratio $\zeta$ for $\tilde{v}_a = \tilde{v}_b = 0.3$ and for different values of the ratio $\rho_C$: $\rho_C = 2$ 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 $\hat{C}_{2222}$ vs. the ratio $\rho_C$ for $\tilde{v}_a = \tilde{v}_b = 0.3$ and for different values of the geometric ratio $\zeta$: $\zeta = 1/10$ 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 $\hat{C}_{2222}$ vs. the geometric ratio $\zeta$ for $\tilde{v}_a = \tilde{v}_b = 0.3$ and for different values of the ratio $\rho_C$: $\rho_C = 2$ red line, $\rho_C = 5$ blue line, $\rho_C = 10$ green line, $\rho_C = 30$ black line, $\rho_C = 50$ violet line.
Figure 5: (a) Dimensionless constant $\tilde{C}_{1212}$ vs. the ratio $\rho_C$ for $\tilde{\nu}_a = \tilde{\nu}_b = 0.3$ and for different values of the geometric ratio $\zeta$: $\zeta = 1/10$ 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 $\tilde{C}_{1212}$ vs. the geometric ratio $\zeta$ for $\tilde{\nu}_a = \tilde{\nu}_b = \tilde{\nu} = 0.3$ and for different values of the ratio $\rho_C$: $\rho_C = 2$ red line, $\rho_C = 5$ blue line, $\rho_C = 10$ green line, $\rho_C = 30$ black line, $\rho_C = 50$ violet line.

Figure 6: (a) Dimensionless constant $\tilde{C}_{1122}$ vs. the ratio $\rho_C$ for $\tilde{\nu}_a = \tilde{\nu}_b = 0.3$ and for different values of the geometric ratio $\zeta$: $\zeta = 1/10$ 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 $\tilde{C}_{1122}$ vs. the geometric ratio $\zeta$ for $\tilde{\nu}_a = \tilde{\nu}_b = 0.3$ and for different values of the ratio $\rho_C$: $\rho_C = 2$ 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. 7 show the variation of the normalized components of the overall thermal dilatation tensor $\tilde{\alpha}_{11}$ and $\tilde{\alpha}_{22}$ as functions of $\rho_C$ and $\rho_a$, assuming $\tilde{\nu} = 0.3$ for both the phases and $\zeta = 1$. In Figs. 8(a) and 9(a) the variation of $\tilde{\alpha}_{11}$ and $\tilde{\alpha}_{22}$ with the non-dimensional ratio $\rho_C$ is reported for several values of $\zeta$ assuming $\tilde{\nu}_a = \tilde{\nu}_b = \tilde{\nu} = 0.3$ and $\rho_a = 2$. 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 $\hat{\alpha}_{iq_1} = 2(\zeta \rho_a + 1)/[(\rho_a + 1)(\zeta + 1)]$ (i.e. $\alpha_{iq_1} = (\alpha_{iq_1}^a + \alpha_{iq_1}^b)/(\zeta + 1)$). In the case where $\rho_C = 1$ and also $\rho_a = 1$, both the elastic and thermal dilatation tensors of the two phases are identical, and then $\hat{\alpha}_{iq_1} = 1$. In Figs. 8(b) and 9(b) the same constants $\hat{\alpha}_{11}$ and $\hat{\alpha}_{22}$ are plotted as functions of $\zeta$ for $\tilde{\nu} = 0.3$, $\rho_a = 2$ and several different values of $\rho_C$. For $\zeta \to 0$, 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 \( \rho_C \) (i.e. \( \tilde{\alpha}_{iq_1} = 2/(1 + \rho_a) \)). This value can be easily derived by using expressions for \( \alpha_{11} \) and \( \alpha_{22} \) reported in Appendix B. Conversely, for \( \zeta \to +\infty \), the thickness of the layer \( b \) tends to zero, the effective thermal dilatation constants tend to those of the phase \( a \) (i.e. \( \tilde{\alpha}_{iq_1} = \alpha_{iq_1}^a \)) and the normalized components \( \tilde{\alpha}_{11} \) and \( \tilde{\alpha}_{22} \) reported in Figs. 8/\( b \) and 9/\( b \) assume the values \( \tilde{\alpha}_{iq_1} = 2\rho_a/(1 + \rho_a) \). 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 \( \rho_a \) with \( \rho_\beta \).

![Diagram](image)

Figure 7: Dimensionless component \( \tilde{\alpha}_{11} \) (a), \( \tilde{\alpha}_{22} \) (b) vs. the ratios \( \rho_C \) and \( \rho_a \) for \( \tilde{\nu}_a = \tilde{\nu}_b = 0.3 \) and \( \zeta = 1/2 \).

The variation of the normalized components of the overall heat conduction tensor \( \tilde{K}_{11} \) and \( \tilde{K}_{22} \) with the non-dimensional ratio \( \rho_K \) are shown in Figs. 10/\( a \) and 11/\( a \). Several values of \( \zeta \) 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 \( \tilde{K}_{iq_1} = \tilde{K}_{iq_1}^b \). In Figs. 10/\( a \) and 11/\( b \) the same non-dimensional components \( \tilde{K}_{11} \) and \( \tilde{K}_{22} \) are reported as functions of \( \zeta \) for different values of \( \rho_K \). As it is shown by these figures, for \( \zeta \to 0 \), \( \tilde{K}_{11} \) and \( \tilde{K}_{22} \) tends to a finite value depending on \( \rho_K \). This limit correspond to the case of vanishing thickness of the layer \( a \), where \( \tilde{K}_{iq_1} = \tilde{K}_{iq_1}^a \), and then \( \tilde{K}_{iq_1} = 2/(1 + \rho_K) \). In the limit \( \zeta \to +\infty \), for which the thickness of the layer \( b \) vanishes and \( \tilde{K}_{iq_1} = \tilde{K}_{iq_1}^b \), 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 \( \rho_K \) with \( \rho_D \).

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Figure 8: Dimensionless component $\tilde{\alpha}_{11}$ vs. the ratio $\rho_C$ for $\tilde{\nu}_a = \tilde{\nu}_b = 0.3$, $\rho_\alpha = 2$ and for different values of the geometric ratio $\zeta$: $\zeta = 1/10$ 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 $\tilde{\alpha}_{11}$ vs. the ratio $\rho_C$ for $\tilde{\nu}_a = \tilde{\nu}_b = 0.3$, $\rho_\alpha = 2$ and for different values of the geometric ratio $\rho_C$: $\rho_C = 2$ red line, $\rho_C = 5$ blue line, $\rho_C = 10$ green line, $\rho_C = 30$ black line, $\rho_C = 50$ violet line.

Figure 9: Dimensionless component $\tilde{\alpha}_{22}$ vs. the ratio $\rho_C$ for $\tilde{\nu}_a = \tilde{\nu}_b = 0.3$, $\rho_\alpha = 2$ and for different values of the geometric ratio $\zeta$: $\zeta = 1/10$ 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 $\tilde{\alpha}_{22}$ vs. the ratio $\rho_C$ for $\tilde{\nu}_a = \tilde{\nu}_b = 0.3$, $\rho_\alpha = 2$ and for different values of the geometric ratio $\rho_C$: $\rho_C = 2$ red line, $\rho_C = 5$ blue line, $\rho_C = 10$ green line, $\rho_C = 30$ black line, $\rho_C = 50$ violet line.
Figure 10: Dimensionless component $\tilde{K}_{11}$ vs. the ratio $\rho_K$ for different values of the geometric ratio $\zeta$: $\zeta = 1/10$ 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 $\rho_K$ for different values of the ratio $\rho_K$: $\rho_K = 2$ red line, $\rho_K = 5$ blue line, $\rho_K = 10$ green line, $\rho_K = 30$ black line, $\rho_K = 50$ violet line.

Figure 11: Dimensionless component $\tilde{K}_{22}$ vs. the ratio $\rho_K$ for different values of the geometric ratio $\zeta$: $\zeta = 1/10$ 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 $\rho_K$ for different values of the ratio $\rho_K$: $\rho_K = 2$ 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 \( L \)-periodic harmonic body forces \( b_i \), directed along the orthotropy direction \( x_j \) (see Fig. 2) and \( L \)-periodic heat and mass sources \( r(x_j) \) and \( s(x_j) \):

\[
\begin{align*}
    b_j(x_j) &= B_j e^{i \frac{2\pi m x_j}{L_j}}, \quad r(x_j) = R e^{i \frac{2\pi n x_j}{L_j}}, \quad s(x_j) = S e^{i \frac{2\pi p x_j}{L_j}}, \\
    \end{align*}
\]

(60)

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 mass concentration 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 fluctuations functions are obtained in exact analytical forms via expressions (53), (54), (55), (57), and (56). Conversely, the solution of the heterogeneous problem with \( L \)-periodic harmonic body forces is computed via FE analysis with periodic boundary conditions on the displacement, temperature and mass concentration fields. For the considered two-dimensional body subject to body forces along the orthotropy axes, heat and mass sources, the homogenized field equations (44), (45) and (46) take the form:

\[
\begin{align*}
    C_{jjjj} \frac{\partial^2 U_j}{\partial x_j^2} - \alpha_{jjj} \frac{\partial \Theta}{\partial x_j} - \beta_{jj} \frac{\partial \Upsilon}{\partial x_j} + b_j &= 0, \\
    K_{jj} \frac{\partial^2 \Theta}{\partial x_j^2} + r &= 0, \\
    D_{jj} \frac{\partial^2 \Upsilon}{\partial x_j^2} + s &= 0, \\
\end{align*}
\]

(61), (62), and (63)

where \( j = 1, 2 \) are not summed indexes. Equations (61), (62) and (63) describe an extensional problem in presence of thermodiffusion. Considering body forces, heat and mass sources of the form (60), the macroscopic displacements, temperature and mass concentration fields are given by

\[
\begin{align*}
    U_j(x_j) &= \frac{B_j L^2}{C_{jjjj}(2\pi m)^2} e^{i \frac{2\pi m x_j}{L_j}} - i \left[ \frac{R \alpha_{jj} L^3}{C_{jjjj} K_{jjj}(2\pi n)^3} e^{i \frac{2\pi n x_j}{L_j}} + \frac{S \beta_{jjj} L^3}{C_{jjjj} D_{jjj}(2\pi p)^3} e^{i \frac{2\pi p x_j}{L_j}} \right], \\
    \Theta(x_j) &= \frac{R L^2}{K_{jjj}(2\pi n)^2} e^{i \frac{2\pi n x_j}{L_j}}, \\
    \Upsilon(x_j) &= \frac{S L^2}{D_{jjj}(2\pi p)^2} e^{i \frac{2\pi p x_j}{L_j}}, \\
\end{align*}
\]

(64), (65), and (66)
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 \( (64), (65) \) and \( (66) \) is accounted. Moreover, the imaginary part of the amplitudes \( B_j, R \) and \( S \) is assumed to be zero. The real part of expressions \( (64), (65) \) and \( (66) \) can be written in the non-dimensional form:

\[
U_j^\alpha(x_j) = \cos\left( \frac{2\pi n x_j}{L_j} \right) + \Xi_j^\alpha \frac{m^2}{2\pi n^3} \sin\left( \frac{2\pi n x_j}{L_j} \right) + \Xi_j^\beta \frac{m^2}{2\pi p^3} \sin\left( \frac{2\pi p x_j}{L_j} \right),
\]

\[
\Theta^\alpha(x_j) = \cos\left( \frac{2\pi n x_j}{L_j} \right), \quad \Upsilon^\alpha(x_j) = \cos\left( \frac{2\pi p x_j}{L_j} \right),
\]

where \( U_j^\alpha = \frac{U_j C_j \pi^m}{B_j L_j^m} \), \( \Theta^\alpha = \frac{\Theta K_j \pi^m}{R L_j} \), \( \Upsilon^\alpha = \frac{\Upsilon D_j \pi^m}{S L_j} \); and \( \Xi_j^\alpha = \frac{\alpha_j RL_j}{K_j B_j} \) and \( \Xi_j^\beta = \beta_j SL_j \). \( j = 1, 2 \) are still not summed indexes.

The amplitude functions \( \Xi_j^\alpha \) and \( \Xi_j^\beta \) are associated respectively with the thermal expansion and mass diffusion contribution to the macroscopic displacement \( \Xi_j \) along the direction \( e_j \). In order to study the influence of the geometrical, elastic and thermodynamic properties of the phases on \( \Xi_j^\alpha \) and \( \Xi_j^\beta \), the following non-dimensional form for these functions is introduced:

\[
\Xi_j^{\alpha, \beta}(\rho_C, \rho_\alpha, \rho_K, \zeta, \nu_\alpha, \nu_K) = \Xi_j^{\alpha, \beta}(\rho_\alpha, \rho_K, \zeta, \nu_\alpha, \nu_K), \quad \text{with } j = 1, 2,
\]

where \( \Xi_j^{\alpha, \beta} = RL_j(\alpha^\alpha + \alpha^\beta)/B_j(K^\alpha + K^\beta) \) and \( \Xi_j^{\beta} = RL_j(\beta^\alpha + \beta^\beta)/B_j(D^\alpha + D^\beta) \). In the case where the two phases possess the same value of the Poisson’s coefficient \( (\nu_\alpha = \nu_\beta) \), the following property is verified for the normalized amplitude functions:

\[
\Xi_j^{\alpha, \beta}(\rho_C, \rho_\alpha, \rho_K, \zeta, \nu) = \Xi_j^{\alpha, \beta}(\rho_\alpha, \rho_K, \zeta, \nu), \quad \Xi_j^{\alpha, \beta}(\rho_C, \rho_\beta, \rho_K, \zeta, \nu) = \Xi_j^{\alpha, \beta}(\rho_\beta, \rho_K, \zeta, \nu).
\]

The three-dimensional plot reported in Fig. \( (12) \) (a) shows the variation of the normalized amplitude component \( \Xi_j^{\alpha, \beta} \) with \( \rho_\alpha \) and \( \rho_K \) for \( \nu_\alpha = \nu_\beta = 0.3 \), \( \rho_C = 10 \) and \( \zeta = 1 \). In Fig. \( (12) \) (b) the same component \( \Xi_j^{\alpha, \beta} \), which represents the contribution of the thermal expansion to the macroscopic displacement along the direction \( e_1 \), is plotted as a function of \( \rho_C \) assuming \( \nu_\alpha = \nu_\beta = 0.3 \), \( \rho_\alpha = 10 \) and several values of the dimensionless ratio \( \zeta \). The variation of the normalized component \( \Xi_j^{\alpha, \beta} \), corresponding to the contribution of the thermal expansion to the macroscopic displacement along \( e_2 \) (see Fig. \( 2 \)), is reported in Fig. \( (13) \) (a) as a function of \( \rho_\alpha \) and \( \rho_K \) for \( \nu_\alpha = \nu_\beta = 0.3 \), \( \rho_C = 10 \) and \( \zeta = 1 \), and in Fig. \( (13) \) (b) as a function of \( \rho_C \) assuming \( \nu_\alpha = \nu_\beta = 0.3 \), \( \rho_\alpha = 10 \). Observing the curves reported in the figures, it can be noted that the normalized amplitude \( \Xi_j^{\alpha, \beta} \), associated to the component of the macroscopic displacement \( U_j^\alpha(x_2) \) parallel to the stratification direction, is greater than the amplitude \( \Xi_j^{\alpha, \beta} \) which correspond to the component \( U_j^\alpha(x_1) \) parallel to the stratification direction. The dimensionless amplitude \( \Xi_j^{\alpha, \beta} \) and \( \Xi_j^{\beta} \), associated to the contributions of the mass diffusion respectively to \( U_j^\alpha(x_1) \) and \( U_j^\beta(x_2) \), are characterized by the same properties of \( \Xi_j^{\alpha, \beta} \) and \( \Xi_j^{\beta} \), and their behavior can be easily studied substituting the non-dimensional ratios \( \rho_\alpha \) and \( \rho_K \) with \( \rho_\beta \) and \( \rho_D \).
Figure 12: (a) Dimensionless amplitude $\tilde{\Xi}_{\alpha 11}$ vs. the ratios $\rho_\alpha$ and $\rho_K$ for $\tilde{\nu}_a = \tilde{\nu}_b = 0.3$, $\rho_C=10$ and $\zeta = 1$. (b) Dimensionless amplitude $\tilde{\Xi}_{\alpha jj}$ vs. the ratios $\rho_C$ for $\tilde{\nu}_a = \tilde{\nu}_b = 0.3$, $\rho_\alpha = \rho_K = 10$ and $\zeta = 1$ for different values of the geometric ratio $\zeta$: $\zeta = 1/10$ red line, $\zeta = 1/5$ blue line, $\zeta = 1$ black line, $\zeta = 5$ blue line points, $\zeta = 10$ red line points.

Figure 13: (a) Dimensionless amplitude $\tilde{\Xi}_{\alpha 22}$ vs. the ratios $\rho_\alpha$ and $\rho_K$ for $\tilde{\nu}_a = \tilde{\nu}_b = 0.3$, $\rho_C=10$ and $\zeta = 1$. (b) Dimensionless amplitude $\tilde{\Xi}_{\beta 22}$ vs. the ratios $\rho_C$ for $\tilde{\nu}_a = \tilde{\nu}_b = 0.3$, $\rho_\alpha = \rho_K = 10$ and $\zeta = 1$ for different values of the geometric ratio $\zeta$: $\zeta = 1/10$ red line, $\zeta = 1/5$ blue line, $\zeta = 1$ black line, $\zeta = 5$ blue line points, $\zeta = 10$ red line points.
The analytical solution (67) and (68), derived by the solution of the homogenized fields equations (61), (62) and (63), 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 \( u_j, \theta, \eta \) which are used together with the up-scaling relations (17) for obtaining the macroscopic fields \( U_j, \Theta, \Upsilon \). These macroscopic quantities are compared with the analytical expressions (67) and (68).

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. 14, the macroscopic displacement component \( U_1^* \) and temperature \( \Theta^* \) evaluated using analytical expressions (67) and (68), 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 \( \Xi_{11}^* = 1 \) (diamonds in the figure). The following values for the geometrical parameters, the ratios between the elastic and of thermodiffusive constants have been assumed:

- \( L/\varepsilon = 10 \)
- \( \rho c = 10 \)
- \( \rho_a = 10 \)
- \( \rho_\beta = 0 \)
- \( \rho_K = 10 \)
- \( \rho = 0 \)

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 \( m, n \) have been introduced. The reported curves show a good agreement between the solution performed by means of the first-order asymptotic homogenization method (continuous lines in the figure) and the results obtained by means of finite element analysis of the heterogeneous problem (diamonds in the figure) is observed.

In Fig. 16, the variation of the normalized component of the macroscopic displacement \( U_1^*(x_1/L) \), temperature \( \Theta^*(x_1/L) \) and mass concentration \( \Upsilon^*(x_1/L) \) 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 \( \nu \) 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 \( \Xi_{11}^* = 1 \), 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. 16(a), (b), for \( \Theta^*(x_1/L) \) in Fig. 16(b) and for \( \Upsilon^*(x_1/L) \) in Fig. 16(d).

The profiles of the macroscopic displacement \( U_2^*(x_2/L) \), temperature in \( \Theta^*(x_2/L) \) and mass concentration \( \Upsilon^*(x_2/L) \) along the characteristic portion of length \( L_2 = L \) are plotted in Fig. 17.
Figure 14: Macroscopic displacement component $U^*_1$ and temperature fields $\Theta^*$ 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 $\Xi_{\alpha 11} = 1$ 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 $\Theta^*$ vs. the ratio $x_1/L$ for different values of wave number $n$ ($n = 1$ red line; $n = 2$, blue line).

Figure 15: Macroscopic displacement component $U^*_2$ and temperature fields $\Theta^*$ due to harmonic body force $b_2$ and temperature source $r$. The heterogeneous model (diamonds) is compared with the homogenized first order model. (a) Dimensionless macro displacement $U^*_2$ vs. the ratio $x_2/L$ for $\Xi_{\alpha 22} = 1$ 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 $\Theta^*$ vs. the ratio $x_2/L$ for different values of wave number $n$ ($n = 1$ red line; $n = 2$, blue line).

as functions of $x_2/L$. Harmonic body forces $b_2(x_2)$, heat and mass sources $r(x_2)$ and $s(x_2)$ and amplitudes $\Xi_{\alpha 22} = 1$ and $\Xi_{\beta 22} = 1$ have been introduced for the numerical solution of the associate thermodiffusive elastic heterogeneous problem. Also in this case, for $U^*_2(x_2/L)$, $\Theta^*(x_2/L)$, and $\Upsilon^*(x_2/L)$, a good agreement between the solution derived by means of the first-order asymptotic homogenization method (continuous lines in the figure) and the results obtained by means of finite element analysis of the heterogeneous problem (diamonds in the figure) is observed.
Figure 16: Macroscopic displacement component $U_1^*$, temperature $\Theta^*$, and mass concentration $\Upsilon^*$ 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 $\Xi^{\alpha}_{11} = 1,\Xi^{\beta}_{11} = 1$ 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 $\Theta^*$ vs. the ratio $x_1/L$ for different values of wave number $n$ ($n = 1$ red line; $n = 2$, blue line). (d) Macro concentration $\Upsilon^*$ vs. the ratio $x_1/L$ for different values of wave number $p$ ($p = 1$ red line; $p = 2$, blue line).
Figure 17: Macroscopic displacement component $U_2^*$, temperature $\Theta^*$, and mass concentration $\Upsilon^*$ due to harmonic body force $b_2$ and temperature and mass sources $r, s$ respectively. The heterogeneous model (diamonds) is compared with the homogenized first order model. Dimensionless macro displacement $U_2^*$ vs. the ratio $x_2/L$ for $\Xi_{22}^a = 1, \Xi_{22}^b = 1$ 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 $\Theta^*$ vs. the ratio $x_2/L$ for different values of wave number $n$ ($n = 1$ red line; $n = 2$, blue line). (d) Macro concentration $\Upsilon^*$ vs. the ratio $x_2/L$ for different values of wave number $p$ ($p = 1$ red line; $p = 2$, blue line).
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. Downscaling relations associating the displacements, temperature and mass concentration 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, mass concentration 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 fields 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 mass concentration fields. Fields 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 mass concentration 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.
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A Symmetry and positive definiteness of elastic and thermodiffusive tensors

In this Appendix, the symmetry properties of the tensors of components \( n_{ijpq}^{(2)} \), \( m_{ijpq}^{(2)} \), \( w_{ijpq}^{(2)} \), and the ellipticity of the fields equations (36), (37), and (38) are demonstrated.

A.1 Symmetry and positive definiteness of tensor of components \( n_{ijpq}^{(2)} \) (vs. \( C_{ijpq} \))

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

\[
\left( C_{ijkl}^{m} n_{kpq1}^{(1)} \right)_{j} + C_{ijkl}^{m} n_{ijpq}^{(1)} = 0,
\]

where \( C_{ijkl}^{m} \) are \( Q \)-periodic functions. The weak form of equation (71), using \( N_{riq2}^{(1)} \) as \( Q \)-periodic test function, is given by

\[
\left\langle \left( C_{ijkl}^{m} n_{kpq1}^{(1)} + C_{ijkl}^{m} n_{ijpq}^{(1)} \right)_{j} N_{riq2}^{(1)} \right\rangle = 0,
\]

applying the divergence theorem to (72), and remembering that for the \( Q \)-periodicity of \( C_{ijkl}^{m} \) and \( N_{riq2}^{(1)} \) the path integrals evaluated on the boundary of the unit cell \( Q \) vanish, we obtain:

\[
\left\langle \left( C_{ijkl}^{m} n_{kpq1}^{(1)} + C_{ijkl}^{m} n_{ijpq}^{(1)} \right) N_{riq2}^{(1)} \right\rangle = 0.
\]

Using the result (73), expression (27) can be written in the equivalent form:

\[
n_{ijpq}^{(2)} = \frac{1}{2} \left\langle \left( C_{ijpq}^{r} + C_{ijpq}^{r} N_{kpq1}^{(1)} \right) + \left( C_{ijpq}^{r} + C_{ijpq}^{r} N_{kpq1}^{(1)} \right) \right\rangle
\]

\[
= \frac{1}{2} \left( C_{ijpq}^{r} + C_{ijpq}^{r} N_{kpq1}^{(1)} \right) + \left( C_{ijpq}^{r} + C_{ijpq}^{r} N_{kpq1}^{(1)} \right) N_{riq2}^{(1)} +
\]

\[
C_{ijpq}^{r} + C_{ijpq}^{r} N_{kpq2}^{(1)} + \left( C_{ijkl}^{m} N_{kpq2}^{(1)} + C_{ijkl}^{m} N_{kpq2}^{(1)} \right) N_{riq2}^{(1)}
\]

\[
= \frac{1}{4} \left\langle C_{ijkl}^{m} \left( N_{riq2}^{(1)} + \delta_{r1} \delta_{j2} + N_{riq2}^{(1)} + \delta_{r2} \delta_{j1} \right) \right\rangle
\]

\[
= \frac{1}{4} \left\langle C_{ijkl}^{m} \left( N_{riq1}^{(1)} + \delta_{r1} \delta_{j1} + N_{riq1}^{(1)} + \delta_{r2} \delta_{j2} \right) \right\rangle
\]

\[
= \frac{1}{4} \left\langle C_{ijkl}^{m} \left( N_{riq1}^{(1)} + \delta_{r1} \delta_{j1} + N_{riq1}^{(1)} + \delta_{r2} \delta_{j2} \right) \right\rangle,
\]

where

\[
C_{ijkl}^{m} = \left[ \begin{array}{cccc}
C_{ijkl}^{m} & 0 & 0 & 0 \\
0 & C_{ijkl}^{m} & 0 & 0 \\
0 & 0 & C_{ijkl}^{m} & 0 \\
0 & 0 & 0 & C_{ijkl}^{m}
\end{array} \right].
\]
as a consequence, we can observe that:

\[ n^{(2)}_{i p q_1 q_2} = \frac{1}{2} (C_{i p q_1 p q_2} + C_{i q_1 q_2 q_2}), \]  

(75)

where the components \( C_{i p q_1 q_2} \) of the overall elastic tensor take the form:

\[ C_{i p q_1 q_2} = \frac{1}{4} \left( C_{r j k l} \left( N^{(1)}_{r i q_2 - j} + \delta_{r i} \delta_{j q_2} + N^{(1)}_{r q_2 i - j} + \delta_{r q_2} \delta_{j i} \right) \cdot \left( N^{(1)}_{k p q_1 - l} + \delta_{k p} \delta_{l q_1} + N^{(1)}_{k q_1 p - l} + \delta_{k q_1} \delta_{l p} \right) \right), \]  

(76)

Observing expression (76), it is easy to deduce that the tensor of components \( C_{i p q_1 q_2} \) is symmetric and positive definite.

### A.2 Symmetry and positive definiteness of tensors of components \( m^{(2)}_{q_1 q_2} \) and \( w^{(2)}_{q_1 q_2} \) (vs. \( K^{(1)}_{q_1 q_2} \) and \( D^{(1)}_{q_1 q_2} \))

Remembering that \( m^{(1)}_{q_1} = 0 \), the cell problems (22), possesses the form

\[ \left( K_{i j}^{m} M_{q_1, q_2}^{(1)} \right)_i + K_{i q_1}^{m} = 0 \]  

(77)

where \( K_{i j}^{m} \) are \( Q \)-periodic functions. The weak form of equation (77), using \( M_{q_2}^{(1)} \) as \( Q \)-periodic test function, is given by

\[ \left\langle \left( K_{i j}^{m} M_{q_1, q_2}^{(1)} + K_{i q_1}^{m} \right), M_{q_2}^{(1)} \right\rangle = 0, \]  

(78)

applying the divergence theorem to (78), and remembering that for the \( Q \)-periodicity of \( K_{i j}^{m} \) and \( M_{q_2}^{(1)} \) the path integrals evaluated on the boundary of the unit cell \( Q \) vanish, we obtain:

\[ \left\langle \left( K_{i j}^{m} M_{q_1, q_2}^{(1)} + K_{i q_1}^{m} \right), M_{q_2}^{(1)} \right\rangle = 0. \]  

(79)

Using the result (70), expression (27) (4) can be written in the equivalent form:

\[ m^{(2)}_{q_1 q_2} = \frac{1}{2} \left( K_{q_1 q_2}^{m} + K_{q_1, q_2}^{m} M_{q_2, q_2}^{(1)} \right) + \left( K_{q_1 q_2}^{m} + K_{q_1, q_2}^{m} M_{q_2, q_2}^{(1)} \right), \]  

\[ = \frac{1}{2} \left( K_{q_1 q_2}^{m} + K_{q_1, q_2}^{m} M_{q_2, q_2}^{(1)} \right) + \left( K_{q_1 q_2}^{m} + K_{q_1, q_2}^{m} M_{q_2, q_2}^{(1)} \right), \]  

\[ = \frac{1}{2} \left( K_{q_1 q_2}^{m} + K_{q_1, q_2}^{m} M_{q_2, q_2}^{(1)} \right), \]  

\[ = \frac{1}{2} \left( K_{q_1 q_2}^{m} + K_{q_1, q_2}^{m} M_{q_2, q_2}^{(1)} \right), \]  

\[ = \frac{1}{2} \left( K_{q_1 q_2}^{m} + K_{q_1, q_2}^{m} M_{q_2, q_2}^{(1)} \right), \]  

(80)

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

\[ K_{q_1 q_2} = \left\langle K_{i j}^{m} (M_{q_2, q_2}^{(1)} + \delta_{q_2}) (M_{q_1, q_2}^{(1)} + \delta_{q_1}) \right\rangle. \]  

(81)
Observing expression (81), 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:

\[
D_{q_1 q_2} = \left\{(D_{ij}^{m}(W_{q_1}^{(1)} + \delta_{q_2})(W_{q_1}^{(1)} + \delta_{q_1}))\right\}.
\]

### B 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:

\[
C_{1111} = \frac{-\zeta^2 \tilde{E}_a \tilde{E}_b + \zeta[(\tilde{E}_a \tilde{v}_a)^2 - 2\tilde{E}_a \tilde{v}_a \tilde{E}_b \tilde{v}_b + (\tilde{E}_b \tilde{v}_a)^2 - (\tilde{E}_a)^2 - (\tilde{E}_b)^2] - \tilde{E}_a \tilde{E}_b}{(\zeta + 1)[\zeta(\tilde{E}_a \tilde{v}_a)^2 - \tilde{E}_a] + \tilde{E}_a(\tilde{v}_b)^2 - \tilde{E}_a};
\]

\[
C_{2222} = \frac{(\zeta + 1)\tilde{E}_a \tilde{E}_b}{\zeta(\tilde{E}_a \tilde{v}_a)^2 - \tilde{E}_a} - \frac{\zeta(\tilde{E}_b \tilde{v}_a)^2 - \tilde{E}_b}{\zeta(\tilde{E}_a \tilde{v}_a)^2 - \tilde{E}_a} + \frac{(\tilde{E}_a)^2 - (\tilde{E}_b)^2}{\zeta(\tilde{E}_a \tilde{v}_a)^2 - \tilde{E}_a} - \frac{(\tilde{E}_a)^2 - (\tilde{E}_b)^2}{\zeta(\tilde{E}_a \tilde{v}_a)^2 - \tilde{E}_a};
\]

\[
C_{1212} = \frac{2[\tilde{E}_a + \tilde{E}_b + \zeta(\tilde{E}_b \tilde{v}_a + \tilde{E}_a)]}{\zeta(\tilde{E}_b (\tilde{v}_a)^2 - \tilde{E}_b) + \tilde{E}_a(\tilde{v}_a)^2 - \tilde{E}_a};
\]

\[
C_{1122} = \frac{\tilde{E}_a \tilde{E}_b (\tilde{v}_a)^2 + \tilde{E}_a(\tilde{v}_a)^2 - \tilde{E}_a}{\zeta(\tilde{E}_b (\tilde{v}_a)^2 - \tilde{E}_b) + \tilde{E}_a(\tilde{v}_a)^2 - \tilde{E}_a} - \frac{\tilde{E}_a \tilde{E}_b (\tilde{v}_a)^2 + \tilde{E}_a(\tilde{v}_a)^2 - \tilde{E}_a}{\zeta(\tilde{E}_b (\tilde{v}_a)^2 - \tilde{E}_b) + \tilde{E}_a(\tilde{v}_a)^2 - \tilde{E}_a};
\]

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

\[
\alpha_{11} = \frac{A_{11} \alpha^a - B_{11} \alpha^a}{\Delta_{11}};
\]

\[
\alpha_{22} = \frac{\zeta(\tilde{E}_b (\tilde{v}_a)^2 - \tilde{E}_b) \alpha^a + \tilde{E}_a((\tilde{v}_b)^2 - 1) \alpha^b}{\zeta(\tilde{E}_b (\tilde{v}_a)^2 - 1) + \tilde{E}_a((\tilde{v}_b)^2 - 1)};
\]

\[
\beta_{11} = \frac{A_{11} \beta^a - B_{11} \beta^a}{\Delta_{11}};
\]

\[
\beta_{22} = \frac{\zeta(\tilde{E}_b (\tilde{v}_a)^2 - \tilde{E}_b) \beta^a + \tilde{E}_a((\tilde{v}_b)^2 - 1) \beta^b}{\zeta(\tilde{E}_b (\tilde{v}_a)^2 - 1) + \tilde{E}_a((\tilde{v}_b)^2 - 1)};
\]

where:

\[
A_{11} = \zeta^2[\tilde{E}_b (\tilde{v}_a)^2 - \tilde{E}_b] + \zeta[\tilde{E}_a (\tilde{v}_b)^2 - \tilde{E}_b \tilde{v}_b + \tilde{E}_b \tilde{v}_b (\tilde{v}_a)^2 + \tilde{E}_a \tilde{v}_a - \tilde{E}_a \tilde{v}_a (\tilde{v}_b)^2 - \tilde{E}_a];
\]

\[
B_{11} = \zeta[\tilde{E}_a \tilde{v}_a (\tilde{v}_b)^2 - \tilde{E}_b + \tilde{E}_b (\tilde{v}_a)^2 + \tilde{E}_b \tilde{v}_b - \tilde{E}_b \tilde{v}_b (\tilde{v}_a)^2 - \tilde{E}_a \tilde{v}_a] + \tilde{E}_a (\tilde{v}_b)^2 - \tilde{E}_a;
\]

\[
\Delta_{11} = (\zeta + 1)[\zeta(\tilde{E}_b (\tilde{v}_a)^2 - 1) + \tilde{E}_a((\tilde{v}_b)^2 - 1)].
\]
Finally, the components of the overall heat conduction and mass diffusion tensors become

\[
K_{11} = \frac{K^b - \zeta K^a}{\zeta + 1}, \quad K_{22} = \frac{(\zeta + 1)K^a K^b}{K^a + \zeta K^b}; \quad (87)
\]
\[
D_{11} = \frac{D^b - \zeta D^a}{\zeta + 1}, \quad D_{22} = \frac{(\zeta + 1)D^a D^b}{D^a + \zeta D^b}. \quad (88)
\]

C Asymptotic expansion of overall elastic and thermodiffusive constants in terms of the phase concentration

In this Appendix, an asymptotic expansion of the overall elastic and thermodiffusive constants of a bi-phase orthotropic layered material, derived in Section 5.1, is performed in terms of the concentration of the two constituent phases. The concentration of the phase \(a\) of the layered media illustrated in Fig. 2 is given by

\[
f_a = \frac{a}{a + b}, \quad (89)
\]

where \(a\) and \(b\) are the thickness of the two distinct phases of the material. The concentration \(f_a\) can be easily expressed as a function of the non-dimensional parameter \(\zeta = a/b\):

\[
f_a = \frac{\zeta}{1 + \zeta}, \quad (90)
\]

and then we have:

\[
\zeta = \frac{f_a}{1 - f_a}. \quad (91)
\]

Substituting (91) into expressions (135), (136), (137), (138) and (139), the overall elastic and thermodiffusive constants of the considered bi-phase orthotropic layered material are expressed as functions of \(f_a\). Performing the asymptotic expansion in terms \(f_a\), the components of the overall elastic tensor become

\[
C_{1111} = C_{1111}^b + \frac{C_{1111}^a C_{2222}^b - C_{1111}^a C_{2222}^b - (C_{1122}^a - C_{1122}^b)^2}{C_{2222}^a} f_a
\]
\[
+ \frac{C_{2222}^a (C_{1122}^a - C_{1122}^b)^2}{(C_{2222}^a)^2} (f_a)^2 + O((f_a)^3); \quad (92)
\]
\[
C_{2222} = C_{2222}^b - \frac{C_{2222}^b (C_{2222}^b - C_{2222}^a)^2}{(C_{2222}^a)^2} f_a + \frac{C_{2222}^a (C_{2222}^a - C_{2222}^b)^2}{(C_{2222}^a)^2} (f_a)^2 + O((f_a)^3); \quad (93)
\]
\[
C_{1212} = C_{1212}^b - \frac{C_{1212}^b (C_{1212}^b - C_{1212}^a)^2}{C_{1212}^a} f_a + \frac{C_{1212}^a (C_{1212}^a - C_{1212}^b)^2}{C_{1212}^a} (f_a)^2 + O((f_a)^3); \quad (94)
\]
\[
C_{1122} = C_{1122}^b + \frac{C_{1122}^b (C_{1122}^b - C_{1122}^a)}{C_{2222}^a} f_a
\]
\[
- \frac{C_{2222}^a C_{1122}^b + C_{1122}^a C_{2222}^b - C_{1122}^a C_{2222}^b - C_{1122}^b C_{2222}^b}{(C_{2222}^a)^2} (f_a)^2 + O((f_a)^3). \quad (95)
\]
The asymptotic expansion of the components of the thermal dilatation tensor \( \mathbf{T} \) and diffusive expansion tensor \( \mathbf{D} \) are respectively given by

\[
\alpha_{11} = \alpha_{11}^b - \frac{C_{1222}^b \alpha_{1222}^a - C_{1222}^a \alpha_{1222}^b}{C_{2222}^a}(f_a)^2 + O((f_a)^3);
\]

\[
\alpha_{22} = \frac{C_{2222}^b \alpha_{22}^b - C_{2222}^a \alpha_{22}^a}{C_{2222}^a}(f_a)^2 + O((f_a)^3);
\]

\[
\beta_{11} = \beta_{11}^b - \frac{C_{1222}^b \beta_{1222}^a - C_{1222}^a \beta_{1222}^b}{C_{2222}^a}(f_a)^2 + O((f_a)^3);
\]

\[
\beta_{22} = \frac{C_{2222}^b \beta_{22}^b - C_{2222}^a \beta_{22}^a}{C_{2222}^a}(f_a)^2 + O((f_a)^3).
\]

Finally, applying the same asymptotic procedure to the components of the heat conduction tensor \( \mathbf{K} \) and mass diffusion tensor \( \mathbf{D} \), we get

\[
K_{11} = K_{11}^b + (K_{11}^a - K_{11}^b)(K_{22}^a)^2 + O((f_a)^3);
\]

\[
K_{22} = K_{22}^b - \frac{K_{22}^b(K_{22}^b - K_{22}^a)}{K_{22}^a}(f_a)^2 + O((f_a)^3);
\]

\[
D_{11} = D_{11}^b + (D_{11}^a - D_{11}^b)(f_a)^2;
\]

\[
D_{22} = D_{22}^b - \frac{D_{22}^b(D_{22}^b - D_{22}^a)}{D_{22}^a}(f_a)^2 + O((f_a)^3).
\]

Similar expressions can be derived for the case of isotropic phases expressing the elastic constants in terms of the Young’s modulus and of the Poisson ratio, and introducing the isotropic thermal dilatation and diffusive expansion coefficients and the isotropic heat conductivity and diffusion coefficients. The overall elastic and thermodiffusive constants associate to an isotropic bi-phase layered material are reported in Appendix B.

It can be easily observed that, as we can expect, for \( f_a = 0 \) expressions (92), (93), (94), (95), and (96) tend to the overall elastic and thermodiffusive constants of the phase \( b \), whereas for \( f_a = 1 \) the same expressions tend to the elastic and thermodiffusive constants of the phase \( a \).
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