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A technique to solve the periodic homogenization problem is described systematically in this work. The method is to solve the cell problems by imposing eigenstrains in terms of thermal or piezoelectric strain to the representative volume element. Homogenized coefficients are then calculated from stress solutions of those cell problems. Benefit of the proposed technique is that it is readily applicable for common finite element softwares regardless of using user subroutines. Several numerical examples are examined. The obtained results show good agreements with the published data.

Keywords: homogenization; composite materials; microstructure; eigenstrain; periodicity

1. Introduction

High-performance composites have been introduced recently, thanks to the modern and effective manufacturing processes [1]. These materials often have multiple phases and complex microstructures. Even when the properties of the constituents are isotropic, the effective behavior of the composite can be anisotropic according to the shape and orientation of the different phases. Generally, the composite materials can thus become strongly inhomogeneous and anisotropic depending on both their complex microstructure and behaviors of the constituents. Characterization of such materials is necessary for the structural design or analysis. Typically, specific experimental tests should be conducted to obtain essential material properties. However, for prediction of a new designed microstructure of composite materials, specimen preparation and testing tasks are always expensive and time consuming. The numerical simulation, as an alternative 'virtual testing' way, can almost promptly provide information about the effective macroscopic properties. A numerical analysis can also predict the overall property variations of the material due to the corresponding material behavior of the constituents and the microstructure architecture parameters [2,3].

Generally, there are two different scales associated with microscopic and macroscopic behaviors to describe a microstructured heterogeneous composite material [4,5]. The first one is a macroscale, denoted by the slowly varying global variable x, at which the heterogeneities are invisible. The other is for the material microarchitecture of heterogeneities' size and

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referred as the microscale, denoted by the rapidly oscillating local variable *y*. To model a structure of such kind of material using the finite element method (FEM), one should utilize models with very fine mesh so that the details at the microscale size of heterogeneities can be captured. That leads to a very expensive computational cost and sometimes it is impossible to perform the analysis due to extremely high requirements of computer resources. Instead, a so-called homogenization process can be used to characterize the heterogeneous material as a homogenized one and then, the equivalent material properties are used in the simulation of the whole structure as in a normal FEM analysis [3].

Homogenization is a process of finding a homogeneous '*effective*' material that is energetically equivalent to a microstructured heterogeneous material [2]. That means, an object of the equivalent homogenized material behaves in the same manner as the original one when it is subjected to usual loadings. Specifically, homogenization method aims to calculate the effective elastic properties of a highly heterogeneous media by averaging over an assumed statistical homogeneous volume. The conditions for such a volume to be chosen as a *Representative Volume Element* (RVE) are sufficiently large at the microscale and sufficiently small at the macroscale and structurally typical of the entire composite material on an average [6]. For a different approach, the RVE size affects the obtained results [7,8]. However, when the ratio of the RVE size to the body dimensions under consideration tends to zero, the results converge to exact solution. Among various approaches to predict the effective properties of composites, the mathematical homogenization method with the periodicity assumption over a *basic cell* (or a representative volume element) is preferable due to its rigorous mathematical background and the ease to implement [3,9,10]. Based on this method, different approaches can be used to obtain the equivalent properties of the highly heterogeneous periodic media. Researches on the homogenization problems are devoted to either making an in-house code [9,10] or writing user-subroutines in commercial softwares [11] to study some particular cases. These approaches, on one hand, are flexible and have facilitated to the researchers and skillful software users, but on the other hand, can be burdensome to the engineers who have less skill.

In the present work, we formulate the homogenization problem for a periodic heterogeneous media and focus on a so-called *eigenstrain technique* to solve the homogenization problems using commercial FEM softwares. The *eigenstrain technique* solves the *basic cell problems* by applying a prescribed eigenstrain as a given local macroscopic scale strain at the material point associating with the basic cell. In cooperation with the commercial FEM softwares, e.g. ANSYS®, MSC PATRAN®/NASTRAN®, MARC®, or the likes, the *eigenstrain technique* can solve the homogenization problems regardless of using any user-subroutine. The method is then used to characterize the mechanical properties of some composite materials having complex microstructures.

The paper is organized as follows: the next section briefly introduces the homogenization problem and its variational formulation; the following section focuses on the background of the eigenstrain method. Section 4 is devoted to examine several numerical examples and to compare the obtained results with the published ones; and finally, the last section presents some discussions and concludes the study in this paper.

2. Formulation of the homogenization problem

Consider a body Ω constituted by a heterogeneous material with the heterogeneities being distributed in a periodic way. A basic cell $\boldsymbol{Y}$ (in microscopic scale) consisting of various phases is a representative of the microstructure of the highly heterogeneous media:

$$\boldsymbol{Y} = \{\boldsymbol{y} \in \boldsymbol{R}^3 : 0 \le y_i \le \mathrm{Y}_i, \quad i = 1,2,3\} \tag{1}$$

Let ε be a small real number and $\varepsilon\boldsymbol{Y} = \{\boldsymbol{x} \in \boldsymbol{R}^3 : 0 \le x_i \le \varepsilon \mathrm{Y}_i, \quad i = 1,2,3\}$ represents the whole space by reproducing the cell $\varepsilon\boldsymbol{Y}$, as shown in Figure 1. Intersection of this infinite medium with a bounded domain of body Ω defines a highly heterogeneous medium because the heterogeneities are $\varepsilon\boldsymbol{Y}$-periodic, where, ε characterizes the ratio between the microstructure scale and the structure scale. In other words, the body under consideration is formed by repeating the microstructure $\boldsymbol{Y}^\varepsilon = \varepsilon \times \boldsymbol{Y}$. The spatial period is described by an element volume $\boldsymbol{Y}^\varepsilon$. Therefore, $\boldsymbol{Y}$ is a reference cell which contains all the relevant information about the microstructure. The mathematical theory of the homogenization method concerns composite media whose microstructure occupies a fixed region with characteristic length ε. It is proved that, as ε goes to zero, the composite structure behaves as it were occupied by an equivalent homogeneous medium and that the actual displacement tends to the homogenized displacement field, which is a solution of the governing equations whose coefficients have been homogenized [5,12].

The stress and strain fields of a periodic heterogeneous media depend on the two variables: $\boldsymbol{x}$ in the macroscopic scale and $\boldsymbol{y}$ in the microscopic scale. They have different values at different locations $\boldsymbol{x}$ in the global sense. However, their local variations – taken into account their dependence on $\boldsymbol{y}$ – are supposed to be periodic [13]. Due to the $\varepsilon\boldsymbol{Y}$ periodicity of geometrical and mechanical properties of the medium, we look for fields in the forms of:

$$\boldsymbol{\sigma}^\varepsilon(\boldsymbol{x}) = \boldsymbol{\sigma}(\boldsymbol{x}, \boldsymbol{x}/\varepsilon) \text{ and } \boldsymbol{e}^\varepsilon(\boldsymbol{x}) = \boldsymbol{e}(\boldsymbol{x}, \boldsymbol{x}/\varepsilon) \tag{2}$$

where, $\boldsymbol{y} \mapsto \boldsymbol{\sigma}(\boldsymbol{x}, \boldsymbol{y})$ and $\boldsymbol{y} \mapsto \boldsymbol{e}(\boldsymbol{x}, \boldsymbol{y})$ are $\boldsymbol{Y}$-periodic functions. Generally, a function $\boldsymbol{y} \mapsto f(\boldsymbol{x}, \boldsymbol{y})$ describes fluctuations of the microscopic field in the $\varepsilon\boldsymbol{Y}$ vicinity of a macroscopic scale point $\boldsymbol{x}$, whereas the macroscopic fields are determined as volume averages over the basic cell $\frac{1}{|\boldsymbol{Y}|}\int_{\boldsymbol{Y}} f(\boldsymbol{x}, \boldsymbol{y}) d\boldsymbol{y}$. The macroscopic stress and strain fields are namely,

$$\sum = \langle \boldsymbol{\sigma}(\boldsymbol{x}, \boldsymbol{y}) \rangle = \frac{1}{|\boldsymbol{Y}|}\int_{\boldsymbol{Y}} \boldsymbol{\sigma}(\boldsymbol{x}, \boldsymbol{y}) d\boldsymbol{y} \quad \text{and} \quad \boldsymbol{E} = \langle \boldsymbol{e}(\boldsymbol{x}, \boldsymbol{y}) \rangle = \frac{1}{|\boldsymbol{Y}|}\int_{\boldsymbol{Y}} \boldsymbol{e}(\boldsymbol{x}, \boldsymbol{y}) d\boldsymbol{y} \tag{3}$$

where, $\langle \bullet \rangle$ stands for the volume averaging operator and $|\boldsymbol{Y}|$ is the volume of the basic cell. The strain is infinitesimal and its components are defined as:

$$e_{ij}(v) = \frac{1}{2}\left(\frac{\partial v_i}{\partial y_j} + \frac{\partial v_j}{\partial y_i}\right) \tag{4}$$

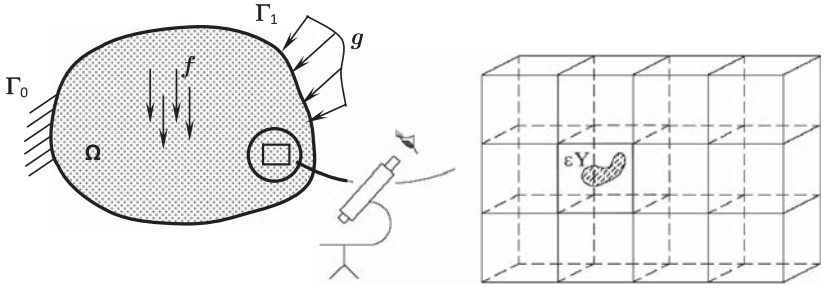


Figure 1. The macroscale and microscale of the homogenization problem.

Using the periodicity conditions, the displacement of the unit cell is decomposed into an average term and a fluctuating term [13]:

$$\boldsymbol{u} = \boldsymbol{E}\boldsymbol{y} + \boldsymbol{v} \text{ or } u_{ij} = E_{ij}y_j + v_i \tag{5}$$

where, $\boldsymbol{E}$ is the prescribed average value of strain field and $\boldsymbol{y} \in \boldsymbol{Y} \mapsto v_i(\boldsymbol{x}, \boldsymbol{y})$ is $\boldsymbol{Y}$-periodic or the fluctuation (oscillatory) term $v_i(\boldsymbol{x}, \bullet)$ takes equal values on the opposite faces of $\partial \boldsymbol{Y}$.

The local strain is also split into its average and a fluctuating term:

$$\boldsymbol{e}(\boldsymbol{u}) = \boldsymbol{E} + \boldsymbol{e}(\boldsymbol{v}) \text{ and } \langle \boldsymbol{e}(\boldsymbol{v}) \rangle = 0 \tag{6}$$

Consequently, the fields of the form $\boldsymbol{y} \in \boldsymbol{Y} \mapsto \boldsymbol{w} = \boldsymbol{E}\boldsymbol{y} + \boldsymbol{v}(\boldsymbol{x}, \boldsymbol{y})$ are called the fields with *periodic deformation*, denoting by the set $\boldsymbol{V}_{\text{per}} = PD(\boldsymbol{Y})$. Then, we have:

$$\boldsymbol{w} \in PD(\boldsymbol{Y}) \;\; \Rightarrow \;\; \langle \boldsymbol{e}(\boldsymbol{w}) \rangle = \boldsymbol{E} \tag{7}$$

Depending upon the condition of the prescribed macroscale quantity, we have two types of approaches: the strain approach and the stress approach. This study only gives the formulation of the homogenization problem using the strain approach in which the macroscale strain is given. The interested reader is referred to [14,15] for the stress approach.

Let $\boldsymbol{a}$ and $\boldsymbol{y}$ be the heterogeneous elasticity coefficients, $\boldsymbol{E}$ be the prescribed macroscopic strain, and the microscopic fields $(\boldsymbol{v}_{\boldsymbol{E}}, \boldsymbol{\sigma}_{\boldsymbol{E}})$ be the solutions of the boundary value problem:

$$(P_{\boldsymbol{E}}) \begin{cases} \boldsymbol{\sigma}_E = \boldsymbol{a}[\boldsymbol{E} + \boldsymbol{e}(\boldsymbol{v}_{\boldsymbol{E}})] \\ div\boldsymbol{\sigma}_{\boldsymbol{E}} = 0 \;\; in \;\; \boldsymbol{Y} \\ v_{\boldsymbol{E}} \;\; \boldsymbol{Y}\text{-periodic; } \boldsymbol{\sigma}_{\boldsymbol{E}}\boldsymbol{n} \text{ antiperiodic on opposite faces of } \partial \boldsymbol{Y} \end{cases}$$

Periodicity is specified as the boundary conditions to make the problem well posed. The problem $(P_{\boldsymbol{E}})$ admits a unique solution (up to a constant field for $\boldsymbol{u}_{\boldsymbol{E}}$) [13], thus the macroscopic stress is determined by $\boldsymbol{\Sigma}^{\boldsymbol{E}} = \langle \boldsymbol{\sigma}_{\boldsymbol{E}} \rangle$

The homogenized elasticity coefficients relate the macroscopic stress and strain:

$$\sum^{E} = a^{\text{hom}}\boldsymbol{E}$$

Because $\boldsymbol{E} \in \boldsymbol{S}^3 = \{3 \times 3 \text{ symmetric matrices}\}$ and if $\{e^i\}_{i=1,2.3}$ is the canonical basis of $\boldsymbol{R}^3$, then the basis tensors of $\boldsymbol{S}^3$ are

$$\boldsymbol{T}^{kl} = \boldsymbol{e}^k \otimes_S \boldsymbol{e}^l = \frac{1}{2}\{\boldsymbol{e}^k \otimes \boldsymbol{e}^l + \boldsymbol{e}^k \otimes \boldsymbol{e}^l\} \quad \text{i.e., } (\boldsymbol{T}^{\boldsymbol{kl}})_{ij} = \frac{1}{2}(\delta_{ij}\delta_{jl} + \delta_{il}\delta_{jk}) \tag{8}$$

where, δ is the Kronecker symbol.

The fluctuating displacement $\boldsymbol{v}^{kl}$ is the solution of the cell problem $(P_{\boldsymbol{T}^{kl}})$, i.e. the microscopic fields $(\boldsymbol{v}^{kl}, \boldsymbol{\sigma}^{kl})$ are induced by the elementary macroscopic strain $\boldsymbol{T}^{kl}$:

$$(P_{\boldsymbol{T}^{kl}})\begin{cases}\boldsymbol{\sigma}^{kl}=\boldsymbol{a}[\boldsymbol{T}^{kl}+\boldsymbol{e}(\boldsymbol{v}^{kl})]\\ div\boldsymbol{\sigma}^{kl}=0 \quad in\ \boldsymbol{Y}\\ \boldsymbol{v}^{kl}\ \boldsymbol{Y}\text{-periodic; }\boldsymbol{\sigma}^{kl}\boldsymbol{n}\text{ anti-periodic on opposite faces of partial }\boldsymbol{Y}\end{cases}$$

By superposition of these elementary solutions, we have $\boldsymbol{v_E}=\boldsymbol{E}_{kl}\boldsymbol{v}^{kl}$. Consequently, the macroscale stress is calculated as:

$$\sum_{ij}^{E}=\langle\boldsymbol{ae}(\boldsymbol{u_E})\rangle_{ij}=\frac{1}{|\boldsymbol{Y}|}\int_{\boldsymbol{Y}}a_{ijpq}e_{pq}(\boldsymbol{Ey}+\boldsymbol{v_E})d\boldsymbol{y}=\frac{1}{|\boldsymbol{Y}|}\left\{\int_{\boldsymbol{Y}}a_{ijpq}\left[(\boldsymbol{T}^{kl}+e_{pq}(\boldsymbol{v}^{kl}))\right]d\boldsymbol{y}\right\}E_{kl}$$
$$=\frac{1}{|\boldsymbol{Y}|}\left\{\int_{\boldsymbol{Y}}a_{ijpq}e_{pq}(\boldsymbol{u}^{kl})\,d\boldsymbol{y}\right\}E_{kl}=a_{ijkl}^{hom}E_{kl}$$

where, a_{ijkl}^{hom} are the homogenized elasticity coefficients and are determined by:

$$a_{ijkl}^{\text{hom}}=\frac{1}{|\boldsymbol{Y}|}\left\{\int_{\boldsymbol{Y}}a_{ijpq}e_{pq}(\boldsymbol{u}^{kl})\,d\boldsymbol{y}\right\}E_{kl}=\langle\boldsymbol{ae}(\boldsymbol{u}^{kl})\rangle_{ij}=\langle a_{ijpq}e_{pq}(\boldsymbol{u}^{kl})\rangle=\langle\sigma^{kl}\rangle_{ij}\tag{9}$$

That means the elasticity coefficients a_{ijkl}^{hom} are the ij-components of the macroscopic stress when the macroscopic strain is $\boldsymbol{T}^{kl}$.

Generally speaking, to obtain the effective mechanical properties a_{ijkl}^{hom} of a periodic heterogeneous material, the solutions of the six cell problems $(P_{\boldsymbol{T}^{kl}})$ are required.

Applying the Green's formula, the variational formulation of the six cell problems $(P_{\boldsymbol{T}^{kl}})$ is given by:

$$(P_{\boldsymbol{T}^{kl}})\begin{cases}\text{Find }\boldsymbol{v}^{kl}\ \boldsymbol{Y}\text{-periodic such that}\\ \int_{\boldsymbol{Y}}\boldsymbol{ae}(\boldsymbol{v}^{kl})\,\boldsymbol{e}(\boldsymbol{\varphi})d\boldsymbol{y}=-\int_{\boldsymbol{Y}}\boldsymbol{ae}(\boldsymbol{\varphi})d\boldsymbol{y}\qquad\forall\boldsymbol{\varphi}\quad\boldsymbol{Y}\text{-periodic}\end{cases}\tag{10}$$

Explicitly, the problem can be rewritten in the matrix form as:

$$\begin{cases}\text{Find }\boldsymbol{v}^{kl}\ \boldsymbol{Y}\text{-periodic such that}\\ \int_{\boldsymbol{Y}}\boldsymbol{e}^{T}(\boldsymbol{\varphi})\boldsymbol{De}(\boldsymbol{v}^{kl})d\boldsymbol{y}=-\int_{\boldsymbol{Y}}\boldsymbol{e}^{T}(\varphi)\boldsymbol{d}_{q}d\boldsymbol{y}\ \ \forall\varphi\ \boldsymbol{Y}\text{-periodic}\end{cases}\tag{11}$$

where, $\boldsymbol{D}=[\,\boldsymbol{d}_1\quad\boldsymbol{d}_2\quad\boldsymbol{d}_3\quad\boldsymbol{d}_4\quad\boldsymbol{d}_5\quad\boldsymbol{d}_6\,]$ is the usual elasticity matrix a_{ijkl} expressed in matrix notation. Applying the finite element technique [10], Equation (11) can be rewritten as:

$$\begin{cases}\text{Find }\boldsymbol{v}^{kl}\ \boldsymbol{Y}\text{-periodic such that}\\ (\int_{\boldsymbol{Y}}\boldsymbol{B}^{T}\boldsymbol{DB}d\boldsymbol{y})\boldsymbol{v}^{kl}=-\int_{\boldsymbol{Y}}\boldsymbol{B}^{T}\boldsymbol{d}_{q}d\boldsymbol{y}\quad q=1,2,...,6\end{cases}\tag{12}$$

in which $\boldsymbol{B}$ is the strain-displacement matrix. One may implement an in-house finite element code to solve Equation (12) and then to compute the homogenized coefficients according to (9) without difficulty [9,10]. Moreover, the user can also develop a user-subroutine in a commercial FEM software environment to solve the above cell problems [11].

If we use a discretization by finite elements of $\boldsymbol{Y}$, it is difficult to get a basis of $\boldsymbol{V}_{\text{per}}=\{\boldsymbol{Y}\text{-periodic fields}\}$. It is more efficient to consider a discretization by finite elements,

say $\boldsymbol{V}^h$, of all the fields defined on $\boldsymbol{Y}$ and to work with $\boldsymbol{V}^h$ and impose periodicity conditions after. Thus, the problem (12) implies a system of Equations (13) and the accompanied periodicity conditions:

$$\boldsymbol{v}^T\boldsymbol{K}\boldsymbol{u} = \boldsymbol{v}^T\boldsymbol{L} \tag{13}$$

Here, $\boldsymbol{K}$ and $\boldsymbol{L}$ are the stiffness matrix and the 'nodal load' vector, respectively. The periodicity conditions of $\boldsymbol{v}^{kl}$ in the cell problems must be imposed through constraint equations to reflect the repeatability of the microstructure. The treatment of such constraint equations can be one of the following: elimination, Lagrange multiplier method, penalty method, and augmented Lagrangian method [16,17]. Commercial FEM softwares always supply utilities to handle with such constraint. The ***CP*** command in ANSYS® and ***MPC*** function in MSC. PATRAN® can be used to define the periodicity conditions. Moreover, for particular problems with symmetric microstructure, only a part of the unit cell is modeled and the periodicity conditions can be reduced to the conventional boundary conditions [10]. A study on alternative methods and comparison of computing time among them can be found in [18]. Method to ensure strain periodicity for a hexagonal unit cell by imposing the kinematic boundary conditions is also introduced [19].

3. The eigenstrain technique

There are several approaches to solve the cell problems, such as implementing a finite element code [9,10], writing a user-subroutine in a commercial FE package, and using special techniques to make the homogenization problems become regular to be solved by FEM. The latter is of interest because it requires less effort and skill to solve the problem with a commercial software at hand. Common techniques in use are the *fictitious volumetric force* method [13,16,20], the *isostrain* (Voigt) method [13,20], and the *isostress* (Reuss) method [13]. Whereas the first one is not suitable for complex microstructured media, the other two do not guarantee the periodicity of the problem. Moreover, the *isostrain* method often overestimates while the *isostress* method underestimates the homogenized properties of a periodic heterogeneous material [13,17]. The technique used in this work, namely the *eigenstrain method*, has a benefit of using a commercial FE package following several simple steps to solve the cell problems instead of implementing a new computer code or writing user-subroutines which are really challenging for practical engineers.

The *eigenstrain* terminology is first defined by Mura [21] to indicate nonelastic strains as thermal expansion, phase transformation, initial strains, plastic strains, etc. The *eigenstrain method* is named due to the fact that this technique solves the basic cell problems of homogenization by applying an *eigenstrain* as a given local macroscopic scale at the material point associating with the basic cell. The fact that the elementary macroscale strain state is achieved by applying an appropriate *eigenstrain* makes this method distinct to the *isostrain method* in which specific displacements are imposed on the boundary to obtain the macroscale strain states. Displacements imposed on the corresponding boundary in the cell problems to achieve the elementary macroscale strain states are:

$$\phi_i^{kl} = \delta_{ik}y_l$$

The corresponding macroscale (average) strain components due to the imposed displacements are given by:

$$\boldsymbol{T}_{ij}^{kl} = \langle \boldsymbol{e}(\boldsymbol{\phi}^{kl}) \rangle_{ij} = \frac{1}{|\boldsymbol{Y}|} \int_{\boldsymbol{Y}} \boldsymbol{e}_{ij}(\boldsymbol{\phi}^{kl}) d\boldsymbol{y} = \frac{1}{|\boldsymbol{Y}|} \int_{\boldsymbol{Y}} \frac{1}{2} \left(\frac{\partial \phi_i^{kl}}{\partial y_j} + \frac{\partial \phi_j^{kl}}{\partial y_i} \right) d\boldsymbol{y} = \frac{1}{|\boldsymbol{Y}|} \int_{\partial \boldsymbol{Y}} \frac{1}{2} (\phi_i^{kl} n_j + \phi_j^{kl} n_i) d\boldsymbol{s}$$

It is worth noting that, for the *isostrain method*, the periodicity condition of the fluctuating displacement in the cell problem does not hold strictly, i.e.

$$\langle \boldsymbol{e}(\boldsymbol{v}^{kl}) \rangle \neq 0$$

This is because the imposed displacements constraint to obtain the elementary macroscale strain and the periodicity condition constraint cannot be applied simultaneously on the same boundary.

To achieve the macroscale elementary strain state and the periodicity condition at the same time, the *eigenstrain method* shows to be a suitable way.

The *eigenstrain* $\boldsymbol{T}^{kl}$ can be either a *thermal strain* as in [22]

$$\boldsymbol{T}^{kl} = \boldsymbol{e}_{\text{thermal}}^{kl} = \boldsymbol{\alpha}^{kl} \Delta T$$

or a piezoelectric strain:

$$\boldsymbol{T}^{kl} = \boldsymbol{e}_{\text{piezo}}^{kl} = \boldsymbol{d}^{kl} \overline{\boldsymbol{E}}$$

where, $\boldsymbol{\alpha}^{kl}$ is the thermal expansion coefficient vector, ΔT is the temperature difference, $\boldsymbol{d}^{kl}$ is the piezoelectric strain matrix, and $\overline{\boldsymbol{E}}$ is the electric field vector. For example, to obtain the macroscale strain state $\boldsymbol{T}^{11}$, the corresponding thermal expansion coefficient is $\boldsymbol{\alpha}^{11} = \{1, 0, 0, 0, 0, 0\}^T$ and the temperature $\Delta T = 1$ if the *eigenstrain* is chosen as a thermal strain. If a piezoelectric strain is applied then the piezoelectric strain matrix is:

$$\boldsymbol{d}^{11} = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}^T$$

and the electric field vector is $\overline{\boldsymbol{E}} = \{1, 0, 0\}^T$. Similarly, the other macroscale strain states can be achieved by applying an appropriate eigenstrain with the corresponding *fictitious material properties* $\boldsymbol{\alpha}^{kl}$ or $\boldsymbol{d}^{kl}$.

In general, the steps to solve the cell problems with a commercial FE software using the *eigenstrain technique* can be summarized as follows:

(1) Build the model of the basic cell.
(2) Define and assign the material properties for each constituent.

(3) Control the meshing process so that nodes located on opposite faces/sides of the cell model are identical .
(4) Apply the periodicity conditions.
(5) Assign the *fictitious material properties* to the whole model to achieve a desired elementary macroscale strain state (the *eigenstrain*).
(6) Solve the problem.
(7) Calculate the homogenized elasticity coefficients using stresses at Gauss points of the elements according to:

$$a_{ijkl}^{\text{hom}} = \frac{1}{|\boldsymbol{Y}|}\int_{\boldsymbol{Y}} \sigma_{ij}^{kl} d\boldsymbol{y} = \frac{1}{|\boldsymbol{Y}|}\sum_{\text{GP}=1}^{\text{NGP}} \sigma_{ij}^{kl}(y_{\text{GP}}) w(y_{\text{GP}}) J(y_{\text{GP}}) \tag{14}$$

where, $\sigma_{ij}^{kl}(y_{\text{GP}})$ is the stress component, $w(y_{\text{GP}})$ and $J(y_{\text{GP}})$ are the weight and Jacobian at the sampling points y_{GP}, respectively.

In the next section, several numerical examples are investigated to validate the proposed technique. The demonstrations are done by using various commercial FE softwares including ANSYS®, MSC. PATRAN®/NASTRAN®, and MARC®. However, other FE packages are applicable to solve the cell problems following the above steps.

4. Numerical examples

4.1. *Example 1: honeycomb microstructure*

A honeycomb microstructure problem is studied as the first benchmark to verify the method and to compare with the published results [10]. Thanks to the symmetry of the problem, only a quarter of the base cell is modeled as shown in Figure 2. The given dimensions are: $a = 3^{-3/4}$ and $t/a = \sqrt{3}/6$. The material is isotropic with Young's modulus $E = 0.91$ and Poisson ratio $\upsilon = 0.3$. All units are assumed consistent. For the sake of simplicity, following notations are used: $a_{1111}^{\text{hom}} = C_{11}$, $a_{1122}^{\text{hom}} = C_{12}$, and $a_{1212}^{\text{hom}} = C_{66}$. The predicted properties using *eigenstrain method* and other methods [9,10] are given in Table 1. As shown in the table, the results of the current method show good agreement with the ones in references.

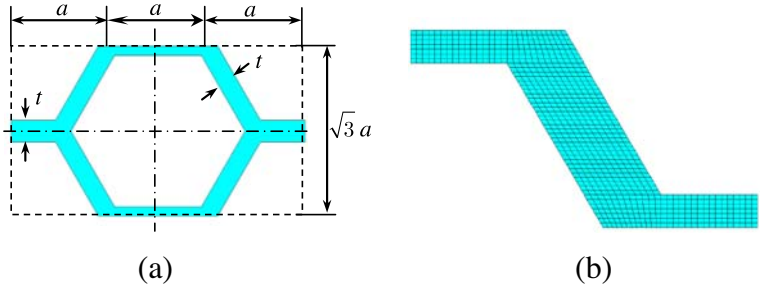


Figure 2. Geometry and FEM model of the unit cell in *Example* 1.

Table 1. Comparison of results in *Example* 1.

	C_{11}	C_{12}	C_{66}
Present study (752 4-node elements)	0.0967	0.0720	0.0123
9072 4-node elements [10]	0.0958	0.0713	0.0125
9520 4-node elements [10]	0.0968	0.0720	0.0124
752 9-node elements [10]	0.0966	0.0720	0.0123

4.2. Example 2: unidirectional fiber-reinforced composite (with a three-dimensional [3D] model)

A three-dimensional (3D) model of the AS4/3501–6 graphite/epoxy unidirectional fiber-reinforced composite material with fiber volume fraction of 60% and the corresponding constituent properties given in Table 2 is studied to compare with Ref. [23]. The FE model of a RVE is shown in Figure 3.

In Ref. [23], the effective elastic moduli of the composites are determined by FE analysis of the RVE using the relation between the average stresses and strains and the strain energy equivalence principle. As shown in Table 3, the obtained properties of the composite materials by the *eigenstrain method* agree very well with the existing predictions and experimental data of [23] and therein references.

4.3. Example 3: 3D nonwoven textile composite

To demonstrate the applicability of the eigenstrain method to a wide range of composite materials, we consider a problem with more complex microstructure, the orthogonal nonwoven composite. Adopting a model from [24,25], the FE model of the unit cell and material properties of constituents are given in Figure 4 and Table 4, respectively.

A good consistency between the obtained solutions in this study and the results from the extended finite element method (X-FEM) or the ones from a study using an in-house FEM code in references is shown in Table 5.

4.4. Example 4: woven composite material

The method is also used to characterize the material properties of a woven composite model and compare with the results given in [26]. The geometrical and material models are shown in Figure 5. The mechanical properties of boron fiber and aluminum matrix are: $E_f = 400$ GPa, $v_f = 0.3$ and $E_m = 72$ GPa, $v_m = 1/3$. A good agreement is obtained between the current study using eigenstrain method and the reference, as shown in (15). The left values are predicted using the current method while the right ones are the average results from the reference [26].

Table 2. Material properties of AS4 and 3501-6.

Material	E_1 (GPa)	E_2 (GPa)	G_{12} (GPa)	υ_{12}	υ_{23}
AS4	235	14	28	0.2	0.25
3501-6	4.8	4.8	1.8	0.34	0.34

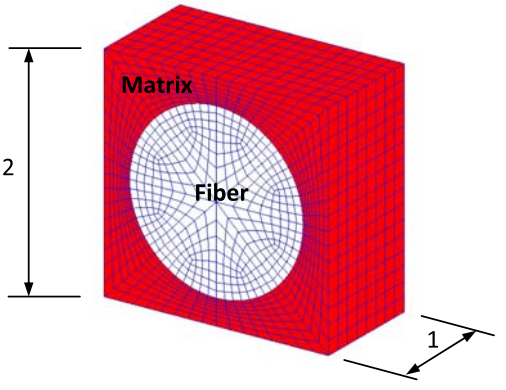


Figure 3. The FE model of the RVE in *Example* 2.

Table 3. Comparison of results in *Example* 2.

	E_1 (GPa)	E_2 (GPa)	G_{12} (GPa)	G_{23} (GPa)	υ_{12}	υ_{23}
Present study	142.8	9.6	6.1	3.2	0.25	0.35
Ref. [23] (FEM)	142.6	9.6	6	3.1	0.25	0.35
Ref. [23] (Experiment)	139.0	9.85	5.25		0.3	

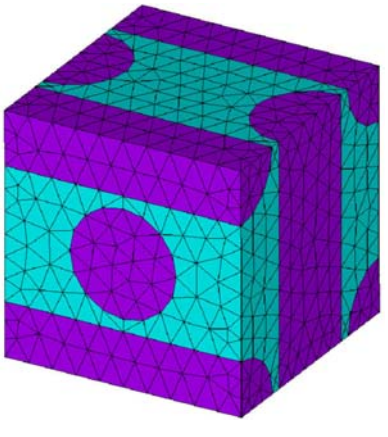


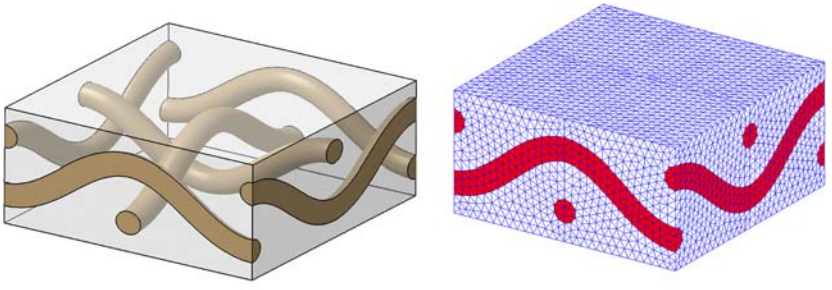
Figure 4. The FE model of a unit cell in *Example* 3.

Table 4. Material properties of constituents in *Example* 3.

Material	E (GPa)	G (GPa)
Fibers	72.0	27.7
Matrix	3.5	1.3

Table 5. Comparison of results in *Example* 3.

	C_{11}	C_{12}	C_{66}
Present study	21	5.4	3.4
X-FEM [24]	21.5	5.6	3.5
FEM code [25]	21.1	5.3	3.4



(a) Geometrical model (b) Finite element model

Figure 5. The geometrical model and finite element model used in Example 4.

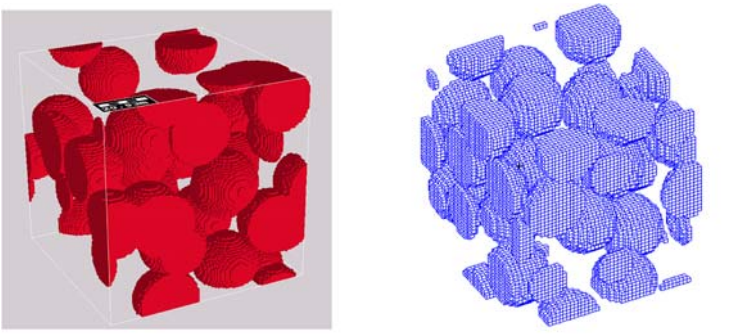
$$[a^{\text{hom}}_{woven}] = \begin{bmatrix} 121.3/120.2 & 58.3/58.0 & 57.4/57.2 & 0/0 & 0/0 & 0/0 \\ 58.3/58.0 & 118.0 & 58.3/58.1 & 0/0 & 0/0 & 0/0 \\ 57.4/57.2 & 58.3/58.1 & 121.3/120.6 & 0/0 & 0/0 & 0/0 \\ 0/0 & 0/0 & 0/0 & 31.4/30.5 & 0/0 & 0/0 \\ 0/0 & 0/0 & 0/0 & 0/0 & 31.4/29.9 & 0/0 \\ 0/0 & 0/0 & 0/0 & 0/0 & 0/0 & 30.4/30.5 \end{bmatrix} \quad (15)$$

4.5. Example 5: composite material with randomly distributed spherical particle

The unit cell model is first generated by GeoDict2009® (licensed by Dr. Andreas Wiegmann at ITWM, Germany, www.geodict.com) and then transferred into the FE environment, e.g. MSC. PATRAN®, as shown in Figure 6. The particle volume fraction is 30%, the radius of particles to unit cell length size ratio is chosen as $L/D = 10/3$ [26]. The material properties of constituents are given in Table 6.

The GeoDict2009® program generates voxel (cubic) elements with the periodic option in x, y, and z direction to guarantee the periodicity constraints of opposite faces. Calculation has been made with different mesh configurations and reported in Figure 7. Due to the random property of the distribution of particles in the model and the usage of voxels to approximate the spherical geometry, the obtained results have a slight difference compared to the referred ones. However, the discrepancy is acceptable, about 7%, 3%, and less than 1% for the $25 \times 25 \times 25$, $50 \times 50 \times 50$, and $75 \times 75 \times 75$ mesh configurations, respectively.

Although the GeoDict2009® model approximates the geometry with certain errors by using voxel elements, we can have a benefit of using such cubic elements. The homogenized coefficients determined by Equation (14) are now evaluated with less effort by using the constant value 1/8 of the element volume for the Jacobian.



(a) The GeoDict2009® model (b) The FE model showing inclusions

Figure 6. The GeoDict2009® model and the FE model of the RVE in *Example* 5.

Table 6. Material properties of constituents in *Example* 4.

	E (GPa)	υ
Particle	450	0.17
Matrix	70	0.3

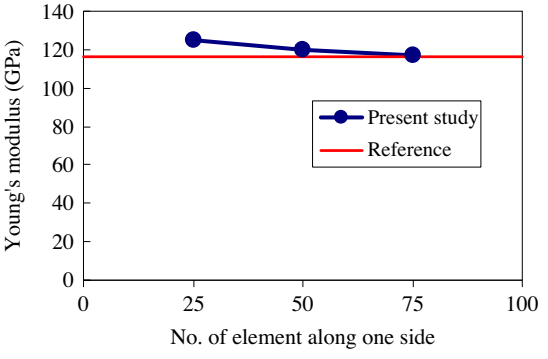


Figure 7. Converged results with respect to the mesh density in *Example* 5.

4.6. Example 6: Glass/alumina two phase material with imperfect bonding

In previous examples, matrix and fiber in the composite are assumed to be perfectly bonded and, therefore, there is no separation between them. However, consideration of the damage of the interface is necessary to accurately predict the behavior of multiple phase composites.

One of the methods to consider the debonding at the interface is to use interface elements (or cohesive elements) which are currently provided in several commercial softwares to simulate the onset and propagation of delamination. These elements have zero thickness and are modeled at the interface of the constituents of a composite material. The constitutive behavior of these elements is usually expressed in terms of tractions vs. relative displacements between the top and bottom edge/surface of the elements (traction-separation curves). Several constitutive laws have been proposed in the literature to express the behavior of these elements [27].

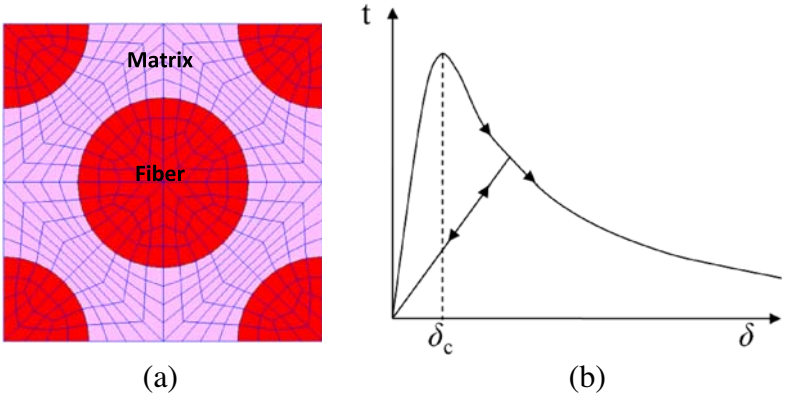


Figure 8. (a) The RVE model in Example 6 and (b) A typical exponential traction–separation curve to model the decohesive phenomenon at the fiber/matrix interface.

In this example we characterize the properties of the glass/alumina composite with consideration of the imperfect bonding of the constituents. The model in this example is based on the reference [28], where the *isostrain method* is used to obtain the homogenized properties. The cohesive elements are modeled along the interface of constituents. A typical FE model of the RVE with the fiber volume fraction of 45% is shown in Figure 8a. The matrix ($E_m = 68$ GPa, $\nu_m = 0.21$) and the fiber ($E_f = 340$ GPa, $\nu_f = 0.24$) are considered as isotropic materials. A typical exponential traction–separation curve, shown in Figure 8(b), is applied for the constitutive behavior of the cohesive elements. The maximum normal traction at the interface is $t_{max} = 1000$ MPa, the corresponding critical normal and shear opening displacement are $\delta_n = \delta_t = 1$ μm. These two cohesive parameters are identified from the experiment work in [28].

An increase of the fiber volume fraction, in a natural way, increases the elastic modulus of the material, as shown in Figure 9. The imperfectly bonded interface made the structure

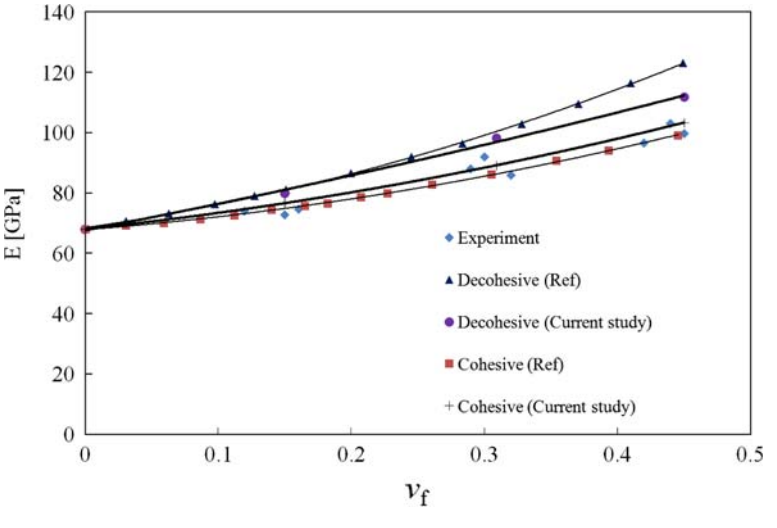


Figure 9. Elastic modulus of the composite with different fiber volume fractions.

softer and, therefore, the predicted modulus is smaller than that in the case of the perfectly bonded interface. When a perfect bonding is assumed, the prediction using the current method and the one in the reference are very close to each other up to a value of the fiber volume fraction about 20%. After that value, the results by the *isostrain method* in [28] are always higher than the predictions by the *eigenstrain method* in this study. The gaps keep increasing when the fiber volume fraction is larger. In the case of the imperfect bonding at the interface, results from the current method and the reference are both well matched to the experimental data.

5. Conclusion

Formulation of the homogenization problem for a periodic heterogeneous media and the *eigenstrain method* to solve such problem has been presented in the current study. This method can be applied with any conventional FE software environment. Several numerical examples have been investigated to verify the method. The results show that the *eigenstrain method* can be effectively used to characterize the mechanical properties of complex micro-structured composites. The main advantages of this method over the others are the simplicity and applicability for engineers and practitioners who have less programming skills. Instead of making an in-house code or implementation of special user-subroutines in FE package, they may use any commercial FE software at hand to characterize the mechanical properties of multiphase composite materials with complex microstructure regardless of handling either advanced tool or programming task.

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