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APPLICATION OF FINITE ELEMENT CODE TO CHARACTERIZE MECHANICAL PROPERTIES OF COMPLEX MICROSTRUCTURED MATERIALS

N.-T. NGUYEN[*], S. KANG[†], D.-Y. KIM[*] AND H. Y. KIM[*]

[*] Department of Mechanical and Biomedical Engineering, Kangwon National University,
192-1, Hyoja2-dong, Chuncheon, Gangwon-do, 200-701, Korea
e-mail: ntnguyen@kangwon.ac.kr, dae-young@kangwon.ac.kr, khy@kangwon.ac.kr
Web page: cae.kangwon.ac.kr

[†] Department of Mechanical Engineering, Yonsei University, Korea
134 Shinchon-dong, Seodaemoon-ku, Seoul, 120-749, Korea
E-mail: snlkang@yonsei.ac.kr

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Abstract. 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 a thermal or a piezoelectric strain to the representative volume element (RVE). Homogenized coefficients are then calculated from stress solutions of those cell problems. As a dual approach, an imposed stress field can also be applied to solve the cell problems. Numerical examples of characterization mechanical properties of complicated microstructure materials are examined. The obtained results show good agreements with the published data. Comparisons show that the technique in this study can be effectively used to characterize the mechanical properties of complex microstructured materials.

1 INTRODUCTION

Mechanical properties of complex microstructured materials can be characterized with the homogenization method which is a process of finding a homogeneous 'effective' material that is energetically equivalent to a microstructured heterogeneous material [1]. That means an object of the equivalent homogenized material behaves in the same manner as the origin one when it is subjected to usual loadings. Specifically, homogenization method aims to calculate effective elastic properties of 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 average [2]. For different approach, the RVE size affects the obtained results [3, 4]. 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 [5-7]. 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 [5, 6] or writing user-subroutines in commercial softwares [8] to study some particular cases. These approaches, on one hand, are flexible and facilitated to the researchers and skillful software users, but on the other hand, can be burdensome to engineers who have less skill.

In the present work we 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 co-operation with commercial FEM softwares, 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.

2 THE HOMOGENIZATION PROBLEM

Generally, there are two different scales associated with microscopic and macroscopic behaviors to describe a microstructured heterogeneous composite material [9, 10]. The first one is a *macroscale*, denoted by the slowly varying *global variables* $\mathbf{x}$, at which the heterogeneities are invisible. The other is for the material micro-architecture of heterogeneities size and referred as the *microscale*, denoted by the rapidly oscillating *local variables* $\mathbf{y}$. 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 [7].

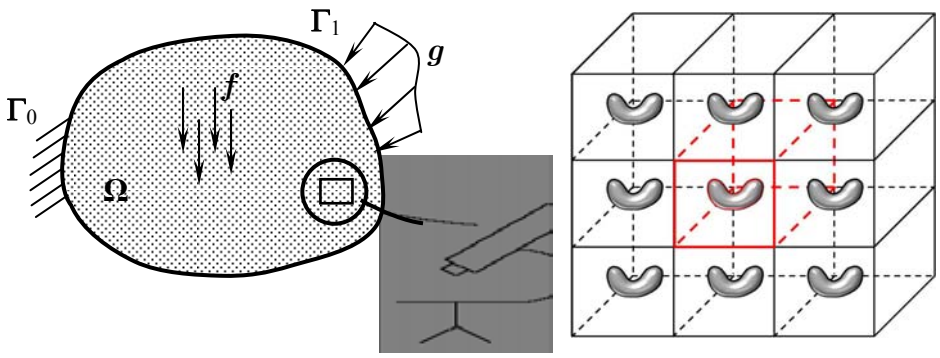


Figure 1: The macroscale and microscale of the homogenization problem

2.1 The problem formulation

From the asymptotic expansion [7, 11], the homogenized elasticity tensor can be determined explicitly by:

$$a_{ijkh}^{\hom} = \frac{1}{|Y|}\int_{Y}\left(a_{ijkh}(\boldsymbol{y}) + a_{ijrs}(\boldsymbol{y})e_{rs}(\boldsymbol{\chi}^{kh})\right)dy \tag{1}$$

where, $\mathbf{Y} = \left\{\mathbf{y} \in \mathbb{R}^n; 0 \le y_i \le Y_i, i = \overline{1,n}\right\}$, $|\mathbf{Y}|$ is the "volume" of the unit cell, $\langle \bullet \rangle = \frac{1}{|\mathbf{Y}|}\int_{\mathbf{Y}}(\bullet)d\mathbf{y}$ denotes the arithmetic mean over the unit cell $\mathbf{Y}$.

χ^{kh} in (1) is the solution of the *cell problem*:

$$\begin{cases} -\dfrac{\partial}{\partial y_j}a_{ijrs}(\mathbf{y})e_{rs}(\chi^{kh}) = \dfrac{\partial}{\partial y_j}a_{ijkh}(\mathbf{y}) \\ \chi^{kh} \text{ is } \mathbf{Y}\text{-periodic} \end{cases} \tag{2}$$

with the periodicity condition defined by: If $\mathbf{y} \in \mathbf{Y} \mapsto v_i(\mathbf{y}) : \mathbf{Y}\text{-periodic}$ or $v_i(\mathbf{y}) \in V_{\text{per}}(\mathbf{Y})$ then $v_i(\mathbf{y})$ takes equal values on the opposite faces of $\mathbf{Y}$.

Generally, we can obtain the solution $\mathbf{v}_E = \chi^{kh}$ by solving the six cell problems and then compute the homogenized elasticity coefficients according to (1). As an alternative, the homogenization problem (2) with periodicity conditions can be formulated in the following forms:

For a given macroscopic strain $\mathbf{E}$,

$$(P_{\mathbf{E}})\begin{cases} Find\ \mathbf{v}_{\mathbf{E}} \in V_{\text{per}}(\mathbf{Y})\ such\ that \\ J_{\mathbf{E}}(\mathbf{v}_{\mathbf{E}}) \le J_{\mathbf{E}}(\mathbf{v}),\ \forall \mathbf{v} \in \mathbf{V}_{\text{per}}(\mathbf{Y}) \end{cases} \tag{3}$$

where $J_{\mathbf{E}}(\mathbf{v}) = \frac{1}{2|\mathbf{Y}|}\int_{\mathbf{Y}}\mathbf{a}(\mathbf{E}+\mathbf{e}(\mathbf{v}))(\mathbf{E}+\mathbf{e}(\mathbf{v}))d\mathbf{y}$

Note that the problems (2) and (3) are equivalent. Moreover, the variational formulation (3) is equivalent to a problem of minimization with constraints:

$$\begin{cases} Find\ \mathbf{v} \in V_{\text{per}}(\mathbf{Y})\ such\ that\ J(\mathbf{v}) \to \min \\ J(\mathbf{v}) = \frac{1}{2}\mathbf{a}(\mathbf{v},\mathbf{v}) - \mathbf{l}(\mathbf{v}) \end{cases} \tag{4}$$

where $\mathbf{a}(\mathbf{v},\mathbf{v}) = \frac{1}{|\mathbf{Y}|}\int_{\mathbf{Y}}\mathbf{a}\mathbf{e}(\mathbf{v}_{\mathbf{E}})\mathbf{e}(\mathbf{v})d\mathbf{y}$; $\mathbf{l}(\mathbf{v}) = -\frac{1}{|\mathbf{Y}|}\int_{\mathbf{Y}}\mathbf{a}\mathbf{E}\mathbf{e}(\mathbf{v})d\mathbf{y}$

Again, by solving 6 problems of formulation (3) or (4) with the imposed macroscopic strains $E_{ij} = (T^{kh})_{ij} = \frac{1}{2}(\delta_{ik}\delta_{jh} + \delta_{ih}\delta_{jk})$, where δ_{ij} is the Kronecker delta symbol; the

homogenized coefficients are determined by:

$$a_{ijkh}^{\hom} = \left\langle \sigma_{ij}^{kh} \right\rangle = \frac{1}{|\mathbf{Y}|} \int_{\mathbf{Y}} \sigma_{ij}^{kh} d\mathbf{y} = \frac{1}{|\mathbf{Y}|} \int_{\mathbf{Y}} \mathbf{a}\left(\mathbf{T}^{kh} + \mathbf{e}\left(\mathbf{v}_{\mathbf{T}^{kh}}\right)\right) d\mathbf{y} \tag{5}$$

2.2 Periodicity conditions

Due to the periodicity of the composites, the microscopic displacement and stress fields are the $\mathbf{Y}$ periodic solution. In the homogenization, the periodic boundary conditions must be imposed on the RVE to reflect the repeatability of the microstructure. For the symmetric inclusion or RVE, the periodic boundary condition leads to the ordinary constraints on the boundary of the RVE [6, 12]. For the non-symmetric inclusion or RVE, appropriate multi-point constraints are imposed on the displacements of nodes on the boundary of RVE in order to produce the periodic boundary conditions [12, 13].

The internal constraints among nodal degrees of freedom can be expressed by a set of constraint equations that must be introduced into the finite element equations. That is, the periodic boundary conditions can be treated as a set of constraint equations. To specify identical displacement for corresponding nodes on opposite edges, the elimination method can be used [12, 14]. The pairs of nodes on the opposite edges of the RVE can be linked by a constraint equation so that the opposite edges have identical deformed shapes. The periodicity conditions can be described by two sets of indices:

$$I^1 = \left\{ i_1^1, i_2^1, ..., i_M^1 \right\}, \qquad I^2 = \left\{ i_1^2, i_2^2, ..., i_M^2 \right\} \tag{6}$$

and a set of M constraint equations:

$$u_{i_k^1} = u_{i_k^2} \qquad k = 1, 2, ..., M \tag{7}$$

The multi-point constrains for RVE can be equivalently expressed in the matrix form by [12]

$$\mathbf{Pu} = \mathbf{0} \tag{8}$$

where $\boldsymbol{P}$ is the transformation matrix whose entries are equal to zero except

$$\begin{aligned} P_{ij} &= 1 \quad \forall i \in I^1 \cup I^2 \\ P_{i_k^1 i_k^2} &= -1 \quad \forall k \in \left\{1, 2, ..., M\right\} \\ P_{i_k^2 i_k^1} &= -1 \quad \forall k \in \left\{1, 2, ..., M\right\} \end{aligned} \tag{9}$$

For the system of N degree of freedom (DOF) with M constraint equations, the resulting transformation matrix should be $N \times \left(N - M\right)$. Figure 2 illustrates the periodicity conditions with constraints on the boundary of the RVE in a 2D case with 2 DOFs at each node. The arrows represent the coupling degrees of freedom for identical nodes on opposite sides. The displacements at corner nodes are fixed.

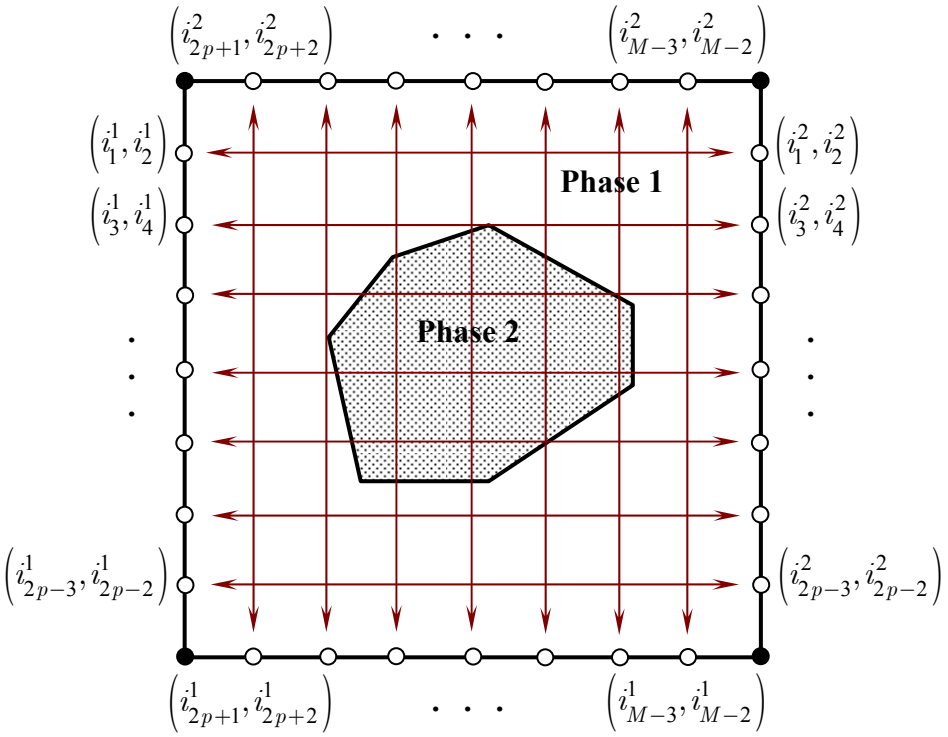


Figure 2: The periodicity constraints on boundary of a 2D RVE

Let u^1 be the free components of $\mathbf{u}$, and u^2, u^3 the components that are linked by the periodicity conditions. Then, we have the cell problem in discretized form:

$$\begin{cases} Find\, \mathbf{u} \in \mathbb{R}^N \; such\, that\, \mathbf{Pu} = \mathbf{0} \; and \\ \mathbf{v}^T\mathbf{Ku} = \mathbf{v}^T\mathbf{L} \quad \forall \mathbf{v} \in \mathbb{R}^N \; such\, that\, \mathbf{Pv} = \mathbf{0} \end{cases} \tag{10}$$

The elimination method to handle the periodicity conditions is easy to implement. However, the bandwidth of the stiffness matrix is seriously increased. It is recommended to use the skyline or sparse storage method for a better computing performance. Commercial FEM softwares 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 [6]. A study on alternative methods and comparison of computing time among them can be found in [15]. Method to ensure strain-periodicity for a hexagonal unit cell by imposing the kinematic boundary conditions is also introduced [16].

2.3 The eigenstrain technique

The eigenstrain terminology is first defined by Mura [17] to indicate non-elastic 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. The displacements imposed on the corresponding boundary in the cell problems to achieve the elementary macroscale strain states are

$$\phi_i^{kl} = \delta_{ik} y_l \tag{11}$$

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

$$\begin{aligned} T_{ij}^{kl} &= \left\langle e\left(\phi^{kl}\right)\right\rangle_{ij} = \frac{1}{|Y|}\int_Y e_{ij}\left(\phi^{kl}\right)dy \\ &= \frac{1}{|Y|}\int_Y \frac{1}{2}\left(\frac{\partial \phi_i^{kl}}{\partial y_j} + \frac{\partial \phi_j^{kl}}{\partial y_i}\right)dy = \frac{1}{|Y|}\int_{\partial Y}\frac{1}{2}\left(\phi_i^{kl} n_j + \phi_j^{kl} n_i\right)ds \end{aligned} \tag{12}$$

It is worth noting that, for the isostrain method, the periodicity condition of the fluctuating displacement in the cell problem doesn't hold strictly, i.e.

$$\left\langle \mathbf{e}\left(\mathbf{v}^{kl}\right)\right\rangle \neq 0 \tag{13}$$

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 at the same time the macroscale elementary strain state and the periodicity condition, the eigenstrain method shows to be a most suitable way. An applied eigenstrain plays the role of the macroscale elementary strain and the periodicity condition discussed in Section 3 will be satisfied by constraining the displacements of nodes on the boundary.

The eigenstrain $\mathbf{T}^{kl}$ can be either a thermal strain as in [18] or a piezoelectric strain:

$$\mathbf{T}^{kl} = \mathbf{e}_{thermal}^{kl} = \boldsymbol{\alpha}^{kl}\Delta T \qquad \text{or} \qquad \mathbf{T}^{kl} = \mathbf{e}_{piezo}^{kl} = \mathbf{d}^{kl}\overline{\mathbf{E}} \tag{14}$$

where $\boldsymbol{\alpha}^{kl}$ is the thermal expansion coefficient vector, ΔT is the temperature difference, $\mathbf{d}^{kl}$ is the piezoelectric strain matrix and $\overline{\mathbf{E}}$ is the electric field vector. For example, to obtain the macroscale strain state $\mathbf{T}^{11}$ the corresponding thermal expansion coefficient is $\boldsymbol{\alpha}^{11} = \left\{1,0,0,0,0,0\right\}^{\mathrm{T}}$ 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

$$\mathbf{d}^{11} = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}^T \tag{15}$$

and the electric field vector is $\bar{\mathbf{E}} = \{1,0,0\}^T$. Similarly, the other macroscale strain states can be achieved by applying an appropriate eigenstrain with the corresponding fictitious material properties $\boldsymbol{\alpha}^{kl}$ or $\mathbf{d}^{kl}$. 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 are identical located on opposite faces/sides of the cell model.
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:

$$\begin{aligned} a_{ijkl}^{\hom} &= \frac{1}{|\mathbf{Y}|}\int_{\mathbf{Y}} \sigma_{ij}^{kl} dy \\ &= \frac{1}{|\mathbf{Y}|}\sum_{GP=1}^{NGP} \sigma_{ij}^{kl}\left(y_{GP}\right) w\left(y_{GP}\right) J\left(y_{GP}\right) \end{aligned} \tag{16}$$

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

3 NUMERICAL EXAMPLES

In this section, two numerical examples are investigated to validate the proposed technique. The demonstrations are done by using various commercial softwares.

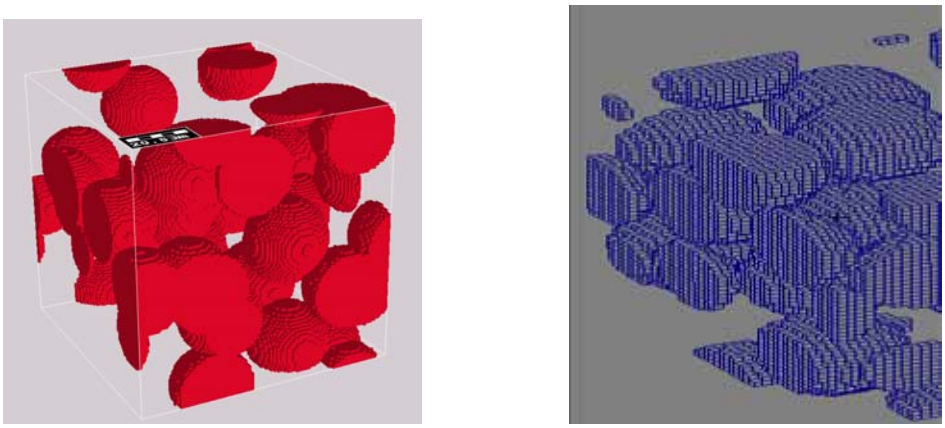
3.1 Composite material with randomly distributed spherical particle

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 3. The particle volume fraction is 30%, the radius of particles to unit cell length size ratio is chosen as $L/D = 10/3$ [19]. The

material properties of constituents are given in Table 1.

Table 1. Material properties of constituents

	E (GPa)	ν
Particle	450	0.17
Matrix	70	0.3



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

Figure 3: The GeoDict2009® model and the FE model of the RVE

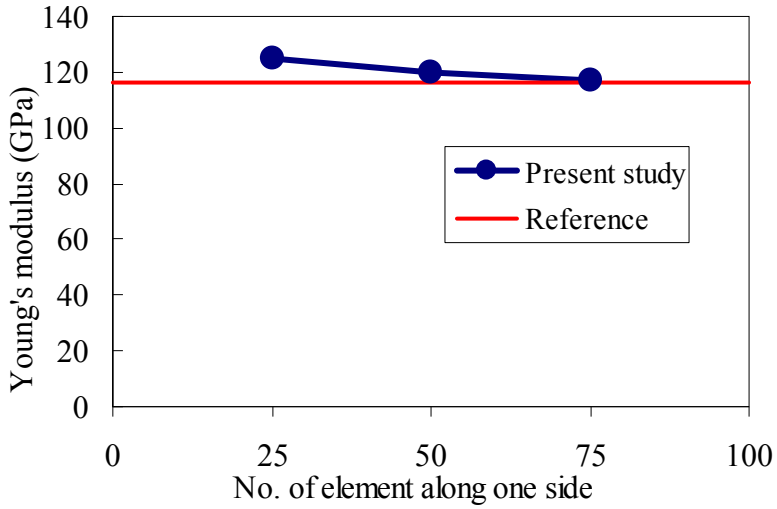


Figure 4: Converged results with respect to the mesh density

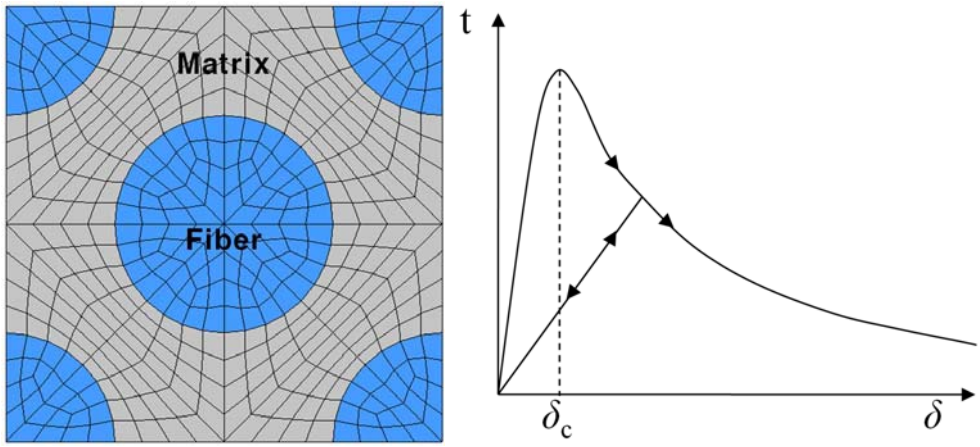
The GeoDict2009® program generates voxel (cubic) elements with the periodic option in x, y and z direction to guarantee the periodicity constraints of opposite faces. Calculation has been made with different mesh configurations and reported in Figure 4. Due to the random property of the distribution 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 25x25x25, 50x50x50 and 75x75x75 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 (16) are now evaluated with less effort by using the constant value 1/8 of the element volume for the Jacobian.

3.2 Glass/alumina two phase material with imperfect bonding

In previous example, matrix and inclusion 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 versus 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 [20].



(a) (b)

Figure 5: (a) The RVE model; (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 [21] 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 5a. 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 5b, is applied for

the constitutive behavior of the cohesive elements. The maximum normal traction at the interface is $t_{\max} = 1000\text{MPa}$, the corresponding critical normal and shear opening displacement are $\delta_n = \delta_t = 1\ \mu\text{m}$. These two cohesive parameters are identified from the experiment work in [21].

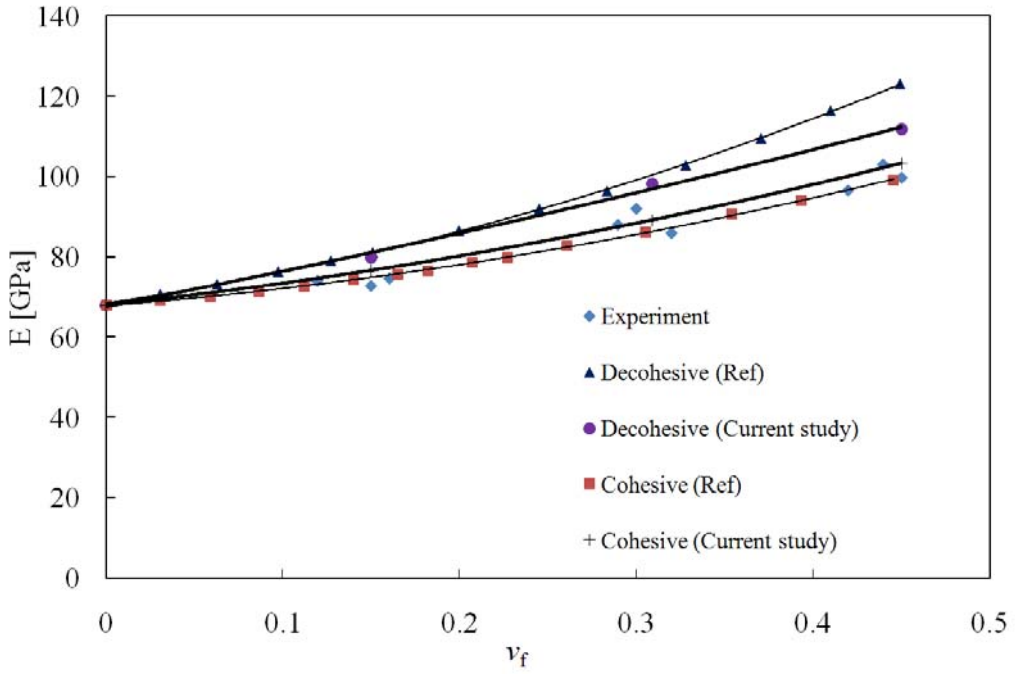


Figure 6: Elastic modulus of the composite with different fiber volume fractions

An increase of the fiber volume fraction, in a natural way, increases the elastic modulus of the material as shown in Figure 6. The imperfectly bonded interface made the structure 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 [21] 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 one are both well matched to the experimental data.

4 CONCLUSIONS

The eigenstrain technique to characterize mechanical properties of complex microstructured materials is presented in the current study. The method can be applied with conventional FE softwares. Numerical examples have been investigated to verify the method. The main advantage of this method is simplicity and applicability for engineers who have less programming skills to use any commercial software at hand to characterize the mechanical properties of multiphase composite materials with complex microstructure regardless of using any user-subroutine.

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