GLOBAL-LOCAL CONSTITUTIVE MODELING OF COMPOSITE MATERIALS BY THE HOMOGENIZATION METHOD

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Abstract: This paper discusses modeling issues in the constitutive relation of a composite material in conjunction with the asymptotic homogenization method. Since the constitutive relations for basic materials of the composite material is given in the microscopic level, the identification of micromechanics and the geometric modeling of the microstructure directly affects the overall mechanical behavior of the structural components. Therefore the modeling in the microscopic level is essential in the analysis of composite materials especially for nonlinear cases. Several numerical examples show that the overall mechanical behavior depends on the constitutive relations defined in the microscopic level as well as the geometry of the microstructure. The FEM-based asymptotic homogenization method and Digital Image-Based (DIB) modeling are utilized to simulate such a global-local nature of the mechanical responses.

Key words: Homogenization method, Composite materials, Constitutive modeling, Geometric modeling, Nonlinear problems.

1 INTRODUCTION

The asymptotic homogenization method has been well-known as a rigorous tool to predict the mechanical behavior of a composite material with periodic microstructure. With the help of the finite element method (FEM), its continuum-based formulation enables the introduction of the various types of constitutive relations for the microstructure as well as geometric configuration (see, for example Guedes and Kikuchi [1] and Léné and Leguillon [2]). However, due to the lack of knowledge about the fundamentals in mechanics of the microstructure or the representative volume elements (RVE), the potential of the homogenization method for nonlinear problems has not been recognized yet.

Recalling the mathematical structure of the homogenized constitutive relation obtained in the asymptotic homogenization [3], the assumptions made for the micromechanical responses and the microstructural geometry can be the source of discrepancy in estimating the overall mechanical behavior of the composite structure. These differences may be negligible in the RVE analysis for linearly elastic composites. However, the effects on the nonlinear behavior of the microstructure should be examined carefully, since the incremental solution method is used to solve the nonlinear equations.

In this paper, we shall examine dependence of the overall mechanical behavior on the constitutive and geometric models of the microstructure. The first part of this paper is devoted to the constitutive modeling within the microstructure in the asymptotic homogenization method. After describing the nonlinear homogenization procedure, several examples of the constitutive relations are presented to demonstrate the global-local nature of mechanical behavior which reflects the constitutive modeling. The second part, discusses the geometric modeling of the microstructure. The specific effects of the geometry on the overall mechanical behavior are examined by showing the microscopic response in the localization process. The arguments made here may be justified in nonlinear computation of the actual microstructural geometry.

2 ASYMPTOTIC HOMOGENIZATION METHOD AND CONSTITUTIVE MODELING

2.1 Homogenization Formulae for Nonlinear Problem

The homogenization formulae for nonlinear problems are derived by utilizing the updated Lagrangian formulation with rate form. Since the macroscopic deformation need not be small even if the microscopic plastic deformation is small, the formulation here is based on the large deformation theory. The boundary value problem in the domain $\Omega$ is posed for a composite structure whose microstructure is assumed to be locally periodic and occupies the domain $Y$. Here the superscript $\varepsilon$ indicates the dependence on the microstructural heterogeneity and relates the microscopic scale $y$ to the macroscopic one $x$ by the relation $x=\varepsilon y$. These variables are used to separate the micro-
and macroscopic problems in the method of two-scale asymptotic expansion.

Since instantaneous linearity is required for the homogenization theory, the constitutive relation considered in this paper is hypo-elastic type, that is, the relative Kirchhoff stress, \( \xi_{ij} \), is related to the strain rate, \( \dot{\varepsilon} \), by the following relation:

\[
\xi_{ij} = E : \dot{\varepsilon},
\]

where \( E \) is the tangent modulus. Noting that the primal variable is a velocity field, we follow the formal procedure in asymptotic homogenization method [3]. Denoting the Cauchy stress in the present step by \( \sigma^0 \), the microscopic problem is given by

\[
\int_Y \sigma^0_{ij} \dot{w}^j dY + \int_Y \nabla \cdot \sigma^0 \dot{w} dY = \int_Y \left[ a(x,y) + \sigma^0_{ij} \right] \dot{w}^i dY - \int_Y \nabla \cdot \sigma^0 \dot{w} dY = 0,
\]

where the variables \( \sigma^0_{ij} \) are called the characteristic deformations and \( w \) is an arbitrary velocity field. Here the coefficient \( b^0 \) is defined as

\[
b^0_{ij} = \frac{1}{2} \left( \delta_{ij} a^0_{mm} \right) + \delta_{ij} \sigma^0_{mm} + \delta_{ij} \sigma^0_{mm} + \delta_{ij} \sigma^0_{mm}.
\]

On the other hand, the macrostructure subjected to the rates of surface traction, \( \dot{t} \), is governed by

\[
\int_{\Omega} a_{ij} \nabla \cdot \dot{u}^0 \dot{w}^j d\Omega + \int_{\partial\Omega} \left( \nabla \cdot \sigma^0_{ij} + \sigma^0_{ij} \cdot \dot{w} + \sigma^0_{ij} \cdot \dot{w} \right) d\Gamma = \int_{\partial\Omega} \dot{t} \cdot \dot{w} d\Gamma,
\]

in which the homogenized Cauchy stress are defined as

\[
\sigma^0_{ij} = \frac{1}{|Y|} \int_Y \sigma_{ij}^0 dY
\]

and \( \sigma^0_{ij} \) has a component such that

\[
a''_{ij} = \left( a_{ij} - a_{ij} \frac{\partial \chi_{ij}}{\partial y_m} - \sigma^0_{ij} \frac{\partial \chi_{ij}}{\partial y_p} \right) dY.
\]

Note that the solution, i.e., the average velocity \( \dot{u}^0 \) is not the function of \( y \) in the homogenized domain \( \Omega \) because of the averaging by \( 1/|Y| \int_Y dY \).

After the solution \( \dot{u}^0 \) of the macroscopic problem is obtained, the microscopic velocity is first obtained as

\[
\dot{w}^i(x,y) = \nabla \nabla \cdot \dot{u}^0_{\omega}.
\]

using both the characteristic deformation and the gradient of \( \dot{u}^0 \). Then the microscopic velocity gradient \( \dot{L}^0 \) and the microscopic strain rate, \( \dot{\varepsilon}^0 \), are respectively obtained as

\[
\dot{L}^0(x,y) = \nabla \cdot \dot{u}^0 - \nabla \cdot \chi^0_{ij} \left( \nabla \cdot \dot{u}^0 \right),
\]

\[
\dot{\varepsilon}^0(x,y) = \epsilon \left( \dot{u}^0(x) - \nabla \cdot \chi^0_{ij} \dot{u}^0(x) \right).
\]

Thus, the stress states are obtained by Eq. (1) and transformed to the Truesdell stress rate:

\[
\dot{S}^0_{ij} = \xi_{ij} - \dot{\varepsilon}^0 \sigma^0 - \sigma^0 \dot{\varepsilon}.
\]

The current states of Cauchy stress and deformations are determined by updating these solutions since we have assumed that the deformation gradient has been assumed to be an identity, namely \( F = I \) in the updated Lagrangian scheme.

For the details of the formulation and computing procedure, one can refer to, for example, Terada and Kikuchi [4]. Using the formulation derived for the micro- and macroscopic problems, we shall describe examples of hypo-elastic constitutive modeling in the next section.

2.2 Examples of constitutive models for the microstructure

As a typical example of composite material, a fiber-reinforced plastic (FRP) is used in the present constitutive modeling for microstructure. Within the framework of hypo-elasticity, various types of micromechanical behavior can be modeled by replacing the tangent modulus in Eq. (1). Elastoplasticity, plastic damage, brittle failure, and nonlinear elasticity are such typical examples. Although the tensor forms are adopted in subsequent sections, each constituent is assumed to be isotropic so that the isotropic plasticity or isotropic continuum damage theory is applicable. Also, the strain defined in the following
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section is understood as the instantaneous (or incremental) values in the nonlinear solution procedure.

Since the failure of the basic materials or interfaces can be recognized as the dissipative phenomena, it seems appropriate to begin with plasticity formulation for the modeling of microscopic failure. Following the J2-flow theory in plasticity, the tangent modulus is defined as

\[ E = E' - \alpha \frac{\partial f}{\partial \sigma^0} \otimes \left( \frac{\partial f}{\partial \sigma^0} \right) \],

(12)

where \( E' \) is the elasticity tensor, \( f \) is the yield function and \( h \) is the hardening modulus. Also, the indicator function \( \alpha \) takes zero when stress state is elastic while it is one when the plastic deformation occurs.

By introducing the damage parameter \( D \) for the elasticity tensor, the following expression describes the mechanical behavior with plastic damage:

\[ E = \bar{E} - \alpha \frac{\partial f}{\partial \sigma^0} \otimes \left( \frac{\partial f}{\partial \sigma^0} \right) - h(\sigma^0) \],

(13)

where \( \bar{E} \) is the damaged elasticity tensor, \( \bar{h} \) the damage hardening parameter and the yield function is re-defined as \( f = f(\sigma, q, D) \). Here, \( q \) are the internal plastic variables and \( \bar{E} \) is defined by

\[ \bar{E} = (1 - D)E' - \frac{H(e)}{e} \sigma^0 \otimes \sigma^0, \]

(14)

where \( H(e) \) is the material parameter which should be determined by experiments and \( e \) is the equivalent strain defined by

\[ e = \sqrt{2W^0(\varepsilon)}, \]

(15)

with the elastic strain energy \( W^0 = 1/2E' : \varepsilon^0 : \varepsilon \). Here, \( E' \) is the undamaged (initial) linear elasticity tensor. The rate expression of damage evolution for isotropic materials is defined by the following flow rule:

\[ \dot{D} = \mu H(e), \]

(16)

where \( \mu \) is a damage consistency parameter that determines damage loading/unloading conditions. These expressions are developed in Simo and Ju [5] based on the strain-based continuum damage theory. On the other hand, brittle failure of constituents can be modeled by changing the damage evolution law without considering plasticity in the above. In this case, denoting the three principal strains by \( \varepsilon_i \) (i=1,2,3), the following damage criterion [6] can be introduced:

\[ \varepsilon^* = \varepsilon_i + \varepsilon_0, \]

(17)

with \( \varepsilon^{'*} > \varepsilon^{*} \) for extension and \( \varepsilon^{'*} < \varepsilon^{*} \) for compression. Here \( \varepsilon^* \) is the damage threshold determined by experiments.

If the nonlinear elastic behavior is assumed for polymeric materials, the extension of the Ramberg-Osgood [6] nonlinear stress-strain relation is possible. That is, the elasticity tensor changing with current stress state is modeled by the following expression:

\[ E = \left[ 1 + n \left( \frac{\sigma}{\sigma_0} \right)^{n+1} \right] \hat{E}, \]

(18)

where \( \sigma_0 \) and \( n \) are the material parameters, \( \bar{\sigma} \) represents the current equivalent stress and \( \hat{E} \) is the initial elasticity tensor observed in experiments.

Using these relations of hypo-elastic constitutive relation in the microscopic level, numerical examples are presented in the following sections to illustrate the dependence of the overall mechanical behavior on the modeling concepts for each basic material in the asymptotic homogenization analysis.

2.3 Numerical examples

Here we examine how the overall constitutive relations are obtained by the homogenization method depending on the assumed nonlinear mechanical behavior of the microstructure. The numerical analyses are carried out by utilizing the examples of constitutive models and the homogenization formulae presented in the above. The unit cell model is assumed to be composed of a single glass fiber and epoxy matrix. The fiber has an idealized circular shape and the volume fraction \( V_f = 40\% \). In order to describe the microstructural response of the FRP, the following four microscopic inelastic phenomena are considered:

1. elastoplasticity in compressive loading
2. elasticity with brittle damage in tensile loading
3. nonlinear elasticity with plastic damage in compressive loading
nonlinear elasticity with brittle damage in tensile loading

Although the fiber part usually has 1.3-times larger strength than matrix, it can be assumed that the fiber does not reveal inelastic behavior such as plasticity in the present deformation range. When the linearly elastic behavior is assumed, Young's moduli and Poisson's ratios are given as follows: $E_f=76$ GPa and $v_f=0.2$ for fiber, and $E_m=4$ GPa and $v_m=0.3$ for matrix. On the other hand, in the nonlinear elasticity case, the initial elasticity constants for matrix part are assumed to be the same as those in linear case and the material constants in Eq. (18) are set to $n=3$ and $\sigma_0=100$ MPa. Also, for the matrix part, the yield stress $\sigma_y=63$ MPa is used to threshold the elastic and perfectly plastic range. Further, the plastic damage with the threshold $\varepsilon=0.006$ is assumed for plastic damage in compression and the brittle damage threshold $\varepsilon^*=0$ for Eq. (18) is introduced only in tensile loading. In all the cases, the interfaces are assumed to be connected elastically for simplicity.

Figure 1 presents the macroscopic stress-strain relationships for the above cases when a unidirectional force is applied in the longitudinal or transverse direction with respect to the fiber alignment. As can be seen from the figure, the different assumptions on the micromechanical behavior provide different nonlinear mechanical behaviors of overall structure. Therefore, if the micromechanical behavior is described correctly, the overall mechanical behavior is obtained directly via homogenization process. In fact, the introduction of brittle damage to the matrix provided very similar results to the actual one reported in the literature [7]. Thus, it is concluded that the actual overall mechanical behavior can be obtained by modeling the constitutive relations for the microstructure.

Once the desired overall response in simple loading case has been obtained by assuming the micromechanical behavior, the same constitutive model in the microscopic level is applicable to the three-dimensional structural analysis by the homogenization method. However, for nonlinear analysis, the microscopic characteristics are dependent of the macroscopic deformation and therefore the microscopic problems have to be solved at every point of the overall structure. As an example of such global-local type computation, we shall consider the unit cell, the overall structure and the boundary conditions shown in Fig. 2. The material properties are the same as in the above and the micromechanical responses (3) and (4) are assumed to be valid. The macro- and microscopic deformations and stress distributions of the overall structure and the unit cell are shown in Fig. 3. Here the unit cell is taken form the upper and lower part of the fixed edge of the structure (point A and B). It can be seen from the fig-
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Fig. 3. Macro-and microscopic deformations along with von-Mises stress distributions (% indicates the ratio to the final deformation).

Fig. 4. Various macroscopic responses in different points.

Fig. 5 (a). Global structure.

(a) Global structure.

(b) Unit cell (50% global deformation).

0 degree-ply

90 degree-ply

0 degree-ply

90 degree-ply

unit cell. In order to obtain the statistical homogeneity of the medium, the unit cell is usually taken a cubic cell with a single inclusion of idealized shape. However, the idealized simplified geometry configuration cause some discrepancy in evaluation of micromechanical responses as well as the homogenized material properties. It is, therefore, necessary to examine the specific effects of microstructural morphology in RVE geometric modeling. Here we shall study such modeling issues in the homogenization method by utilizing the Digital Image-Based (DIB) modeling technique, which was originally developed by Hollister and Kikuchi [8] to include the geometric complexity of bone microstructure in bioengineering.

The DIB modeling technique can realize the accurate geometry of the microscopic heterogeneity. Since the FE model obtained in this technique is the direct interpretation of two dimensionally represented micrograph of a real composite material by the image processing software, the homogenization analyses by the FEM can reflect the specific effects of the actual geometric configuration. The details of the DIB modeling procedure and its applications are found in [9].

In order to illustrate the capability of the method for studying the effects of microstructural geometry, let us consider four types of fiber-shapes (Fig. 5 (a)). The fiber shapes is changed by the drawing software and then the image processing techniques such as thresholding or adjusting are used for all the models to have the same volume fractions (Vf=0.27). For the sake of simplicity, the homogenization for linear elasticity [1] is used in this analysis and the same elasticity constants are used for the matrix and embedded fiber parts as in Subsection 2.3. Figure 5 (b) shows the microscopic von-Mises stress within the unit cell that is the localized response to the 0.1%-

3 GEOMETRIC MODELING OF MICROSTRUCTURE

3.1 Homogenization analysis with the DIB modeling technique

In the homogenization theory, the periodic distribution of the RVE is assumed and therefore the RVE is called the
macroscopic tensile strain in x- (transverse) direction to the fiber. Although the overall homogenized elasticity constants do not reveal significant difference (less than 1%), the patterns and values of stress concentration observed from the figure are completely different. The DIB modeling makes it easy to capture such effects in the homogenization analyses.

While the phase interactions can be accurately evaluated by keeping the accurate microstructural geometry, the interaction between neighboring inclusions are taken into account if the unit cell is simplified to have two inclusions (Fig. 6(a)). The material constants used in the matrix/fiber phase are the same as before and all the fiber-volume fractions are set to be equal ($V_f=0.2$). In spite of their morphological differences, each homogenized elasticity constraint has less than 1%-difference from others. In contrast, the trend does not apply for microscopic stress distribution; Figure 6(b) illustrates significant differences between their microscopic responses. Here the microscopic stress distribution were obtained by applying the 0.1%-macroscopic strain in x-direction. Thus, the idealization of the microstructural geometry cause more severe error in evaluating the microscopic stress than in estimating the homogenized material properties.

In order to study quantitatively the dependence of the micromechanical behavior on the model geometry, let us define the following stress mismatch between two phases

$$F = \left| \langle \sigma_m \rangle - \langle \sigma_f \rangle \right|, \quad (19)$$

where $\langle \sigma_m \rangle$ indicates the von-Mises stress of matrix phase averaged over the matrix and $\langle \sigma_f \rangle$ is defined for the fiber part in the same way. The value of stress mismatch with respect to the relative distance of inclusions shown in Fig. 7. As can be seen from the figure, the microscopic stress values are disturbed from the equally spaced inclusions, i.e., they are affected by the mutual positions of inclusions. Therefore, such a morphological effects must be taken into account in the homogenization analysis.

It is found that the DIB modeling and image processing technique can deal with complicated microstructural geometry so that the specific morphological effects can be considered. It is therefore expected that the microscopic deformations obtained by the localization are more accurate than the usual FE geometry modeling. The examples presented here were simple, but illustrative for studying...
the effects of microstructural morphology as well as the constitutive relations.

3.3 Geometric effects in the nonlinear homogenization method

Within the linear elasticity framework, the effects of microstructural geometry on both macro- and micromechanical behavior of composites are not so important from a practical point of view. Although the results themselves are applicable in designing composite material based upon the micromechanical responses, it is suggested that the evaluation of microscopic stress is critical in nonlinear problems such as elastoplasticity. When the nonlinear deformation of overall structure is computed by the incremental solution method, the values of microscopic stress in a certain increment are used as initial values in the next increment. Therefore, the microstructural geometry must be modeled correctly so that the microscopic stress and hence the macroscopic deformation are evaluated accurately. The objective here is to demonstrate the importance of the geometric modeling of the unit cell in the nonlinear homogenization. While the successive evaluation of the macro- and microscopic variables is demonstrated by the incremental solution method, the dependence of the global-local nonlinear mechanical behavior on the RVE geometric modeling is examined.

![Fig. 8. Micrograph of SiC-reinforced MoSi2 composite.](image)

![Table 1. Material properties of the MMC.](table)

<table>
<thead>
<tr>
<th>Phase</th>
<th>Young's modulus, GPa</th>
<th>Poisson's ratio</th>
<th>Yield stress, MPa</th>
<th>Hardening parameter</th>
</tr>
</thead>
<tbody>
<tr>
<td>Matrix</td>
<td>400</td>
<td>0.20</td>
<td>300</td>
<td>0.2</td>
</tr>
<tr>
<td>Inclusion</td>
<td>450</td>
<td>0.25</td>
<td>-</td>
<td>-</td>
</tr>
</tbody>
</table>

The metal matrix composite (Mo2Si-SiC) presented in Fig. 8 is used to obtain the overall mechanical response to unidirectional tensile force and elastoplasticity with large deformation is assumed as the mechanical behavior of

![Fig. 9. Unit cell models of the MMC.](image)

![Fig. 10. Macroscopic unidirectional response of the MMC.](image)

Mo2Si-matrix phase. The material constants of each phase are given in Table 1. In order to see the effects of geometric modeling, two kinds of the 3D unit cell model are used in this nonlinear homogenization method; one is constructed by usual FE meshing and the other by the DIB modeling technique and image processing [9] (see Fig. 9), both of which reveal isotropy in linear elasticity range.

The macroscopic stress-strain curves are presented in Fig. 10 to illustrate the influence of geometry of the unit cell model. It can be seen from the figure that the idealized model is slightly stiffer than the digitized one in linear elastic range.

Although the direct comparison is difficult because the order of FE approximation is different, the qualitative discussion may be possible. That is, the number of elements to model a single fiber in the idealized model is much larger then that of the digitized model. This implied that if the digitized model has the same order of FE approximation as that of the idealized one to represent the heterogeneity, the elasticity response becomes more compliant. Then onset of the microscopic plastic yielding will be delayed and therefore the trend of the strain hardening would be different. This is also confirmed from the equivalent plastic strain distribution when the plastic deformation begins (Fig. 11). The plastic yielding occurs in several local regions and propagates gradually within the unit cell. Furthermore, since the unit cell size is not so large that the volume element could not be a representa-
tive, the microscopic variables such as stress is not accurately evaluated in each increment. Thus the actual stress-strain curve for the digitized unit cell model is probably quite different from that of the idealized one.

In summary, the constitutive modeling of the asymptotic homogenization method provides the accurate evaluation of the nonlinear global-local deformation of a composite material only when the microstructural geometry of composites is appropriately modeled.

![Figure 11](image) Onset of the plastic yielding with the unit cells.

4 CONCLUDING REMARKS

The modeling issues in the constitutive relation for a microstructure and the microstructural geometry were discussed in conjunction with the RVE homogenization analysis. Although the influences may be small in linear elasticity framework, the analysis for nonlinear mechanical behavior of composites suffer from the errors due to the irrelevant approximations in the modeling.

The macroscopic (global) mechanical response is obtained as the asymptotic behavior of the constitutive relation which is defined in the microscopic (local) level. Depending on the assumed micromechanical responses of individual phases, the completely different overall mechanical behavior can be obtained. It was also found that the geometric modeling of the microstructure influences the micromechanical response as well as overall mechanical behavior. That is, by taking the unit cell model such that contains enough information about the heterogeneities of the composite, the homogenization analysis can prevent from having significant error in predicting the mechanical behavior of the composite material.

In conclusion, since the asymptotic homogenization method enables the construction of the global-local estimates on the nonlinear mechanical behavior of a composite material, much more attention must be paid to both the constitutive relation that describes the microscopic mechanism within the RVE and the geometric modeling in the FEM-based asymptotic homogenization method.

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