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The formulation of homogenization method applied to large deformation problem for composite materials

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Abstract

In order to analyze the mechanical behaviors of composite materials under large deformation, the formulation of the homogenization method is described. In this formulation, assuming that the microstructures in a local region of the global structure are deformed uniformly and that consequently the microscopic periodicity remains in the local region under large deformation, the microscopic deformation is precisely defined by the perturbed displacement and product of macroscopic displacement gradient and microscopic coordinates. Finally, microscopic and macroscopic equations are obtained. The above mentioned assumption of the periodicity of microstructures is experimentally validated. The computer program is also developed according to this formulation, and the large deformation is analyzed for the unidirectional fiber reinforced composite material and the knitted fabric composite material. © 2000 Elsevier Science Ltd. All rights reserved.

Keywords: Homogenization method; Composite material; Large deformation; Microstructure

1. Introduction

In recent years, the composite materials are used in many engineering fields. The characteristics of the composite materials depend on the microscopic architecture. Thus, micro-macro coupled problems are becoming an important issue in such fields as applied mathematics, applied mechanics and computational mechanics. Since the final goal is to design the macroscopic properties and functions to meet the requirements, the microscopic heterogeneity has been folded in equivalent macroscopic properties so far by the rule of mixture, equivalent inclusion method using Eshelby tensor or RVE

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(Representative Volume Element) method (Hashin, 1983) etc. In 1990s, after the paper by Guedes and Kikuchi (1990), the homogenization method is a matter of concern and interest not only in the computational mechanics field but also in the materials science field.

The basic theory of the homogenization method can be found in the papers published in 1970s and early 1980s, for instance, by Babuska (1976), Cioranescu and Paulin (1979), Sanchez-Palencia (1980), Lions (1981), Bakhvalov and Panasenko (1989) and many applied mathematicians. Guedes and Kikuchi (1990) has developed a new formulation of this method in a weak form and shown a guideline for numerical analysis to engineers. Also, practical applications of this method to the analysis of composite materials have been reported. Duvaut and Nuc (1983) applied it to the unidirectional fiber reinforced composite material, Lene and Leguillon (1982) considered the slip at the fiber/matrix interface, Shkoller and Maewal (1996) considered defective region like resin-rich region in fiber tow, and Bigourdan et al. (1991) as well as Takano and Zako (1995a) applied it to woven fabric composite materials. Many other studies are also found to enhance the homogenization method to solve other problems than the above elastic problem. Thermoelastic problem was solved by Francfort (1983), steady-state creep problem by Aravas et al. (1995), time-dependent creep problem by Wu and Ohno (1997), elasto-plastic problem by Jansson (1992), Terada et al. (1995, 1996) and Ghosh et al. (1996), and solid-fluid mixture problem by Terada et al. (1998). The authors Takano and Zako (1995b, 1996a) presented a formulation with initial stresses and solved a large deformation problem and damage propagation problem by a step-wise linear algorithm. In summary, the challenge to extend the homogenization method to solve various nonlinear problems has been carried out in 1990s. However, the application of this method to large deformation problem has remained an open problem till date. We can find only few literatures on the large deformation analysis by the homogenization method, such as a paper by Terada et al. (1995, 1996) and another by Okada et al. (1998). In analyzing the large deformation problems, it is necessary to update both macro- and microscopic models. However, because they did not describe the microscopic deformation, the update of the microstructure under large deformation was not clearly discussed.

Therefore, the purpose of our study is to present a new formulation of the homogenization method for large deformation analysis of composite materials with clear definition of the microscopic deformation. Assume that the microstructures are very small compared with the global body, and are periodically arrayed. Assume a local region such as a discretized finite element which is also small compared with the global body, and assume that the microstructures are periodically arrayed in that region. When the load is applied to the body and it is largely deformed, we assume that the periodicity remains in the local region even after deformation as shown in Fig. 1. In this problem setting, the homogenization method seems to be applicable to large deformation problems similar to the conventional applications to the linear problem. In other words, the local region can be replaced to a homogenized model. As shown in Fig. 1, in general, the deformation of the microstructures in one small region is different from that in other region. Hence, the formulation of the homogenization method applied to large deformation problem should be carried out for the local region and the microstructures in it. As mentioned above, we can suppose the local region is a part of the macroscopic body and it can be replaced to a homogenized model. Using the finite element method (FEM) to solve the derived partial differential equations, the local region is regarded as an element. If we define the microstructure element by element and update the microstructures during the large deformation for all the elements, we can solve the large deformation problem by the micro-macro modeling and the homogenization formulation proposed in this paper.

Experimental investigation to prove the validity of above mentioned problem setting was also conducted for a knitted fabric composite thermoplastics. In recent years, applications of knitted fabric composite materials are investigated, for example, to vehicle door by Kim et al. (1995) and biomaterial by Ramakrishna et al. (1997a). Other research works on the forming processes are also found that lead to obtain products with a variety of shapes, such as the deep-draw forming process investigated by



Nishiyabu (1995). In such forming process, large deformation occurs both macroscopically and microscopically. Understanding of the properties under large deformation is essential. Experimental works to measure the mechanical properties of these materials have been reported by many researchers, for example, Gommers et al. (1995) or Mayer et al. (1998). Ramakrishna (1997b) has proposed a cross-over model for the knitted fabric composite material to estimate the homogenized elastic modulus, which is one of the mechanical approaches based on the geometric information of the knitted fabrics. If largely deformed microstructures are known by experimental observation, his model is very convenient and effective. On the contrary, we take a mathematical approach, and the emphasis is put on the numerical prediction of the large deformation of microstructures under arbitrary macroscopic boundary conditions for arbitrary composite materials with complex microstructures.

2. Formulation

This section describes the formulation of the homogenization method applied to large deformation problem of an elastic body. First, we describe the large deformation theory. Next, using two different coordinate systems, i.e., macroscopic coordinate X and microscopic coordinate Y, the displacement is divided into a uniform displacement and a perturbed one caused by microstructural heterogeneity. Then, similar to the formulation of conventional linear homogenization theory, such as using the averaging principle, the formulation of the homogenization method applied to large deformation problem is derived.

2.1. Large deformation theory

The equilibrium equation for a three-dimensional elastic body is written as Eq. (1). X denotes the undeformed configuration at the initial time.

$$\frac{\partial \Pi_{ji}}{\partial X_j} + b_i = 0 \tag{1}$$

where Π is first Piola-Kirchhoff stress with respect to the initial configuration and b is the body force. Making the time derivation of Eq. (1), and applying the virtual displacement method using the divergence theorem, Eq. (2) is obtained. This is the principle of virtual work expressed in rate form

$$\int_{\Omega} \dot{\Pi}_{ji} \frac{\partial \delta u_i}{\partial X_j} \, \mathrm{d}\Omega = \int_{\Omega} \delta u_i \dot{b}_i \, \mathrm{d}\Omega + \int_{\Gamma} \delta u_i \dot{t}_i \, \mathrm{d}\Gamma \quad \forall \delta u \tag{2}$$

b is the rate of body force and \dot{t} is the rate of traction on the boundary Γ . The constitutive equation is expressed by

$$S_{ij} = C_{ijkl} \dot{E}_{kl} \tag{3}$$

where \dot{S}_{ij} is the rate of second Piola–Kirchhoff stress and \dot{E}_{kl} is the rate of Green–Lagrange strain. By substituting Eq. (3) into Eq. (2) and applying the updated Lagrangian formulation, we obtain the following equation (4)

$$\int_{\Omega} \frac{\partial \delta u_i}{\partial X_j} (C_{ijkl} + \delta_{ik} S_{jl}) \frac{\partial \dot{u}_k}{\partial X_l} \, \mathrm{d}\Omega = \int_{\Omega} \delta u_i \dot{b}_i \, \mathrm{d}\Omega + \int_{\Gamma} \delta u_i \dot{t}_i \, \mathrm{d}\Gamma \quad \forall \delta u \tag{4}$$

The stress S_{il} in Eq. (4) can be approximated by the stress at the initial state of each step. At the first

step, Eq. (4) becomes a linear equation, because the stress at the initial state of the first step is zero. The above equations are described only in the coordinate system X.

2.2. Displacements of global structure and microstructure

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Suppose a three-dimensional elastic body is the assembly of periodic microscopic structures and assume one local region. Also assume that the periodicity of the microstructures exists in the local region during the deformation, and the local region can be replaced to the homogenized model. Hence, as in Fig. 1, we consider two coordinate systems, i.e., macroscopic coordinate system X and microscopic corrdinating system Y, which are related by the scale ratio ε as follows

$$\mathbf{y} = \mathbf{x}/\varepsilon \tag{5}$$

 $\mathbf{x} = (x_1, x_2, x_3)$ is written in the macroscopic coordinate system X, and $\mathbf{y} = (y_1, y_2, y_3)$ in the microscopic Y. X is used to describe the global structure as well as the local region, while Y is used to describe the microstructure. When we assume that the microstructure is very small compared with the global structure as well as the local region, the scale ratio ε is a very small number. When the load is applied to the body and is largely deformed, the deformation of the microstructure in one small region is different from that in the other. However, we can consider that the periodicity remains in the local region even after deformation as shown in Fig. 1. In this case, the microstructures in that region are assumed to be deformed uniformly. Therefore, we consider the homogenized (or macroscopic) model of that region, and the rate of displacement in the homogenized region can be described as Eq. (6)

$$\dot{u}_i^{\rm H}(\boldsymbol{x}) = \dot{\alpha}_{ij}^{\rm H} x_j + \dot{u}_i^{\rm H}(0) \quad \left(\dot{\alpha}_{ij}^{\rm H} \text{ is constant}\right) \tag{6}$$

where $\dot{u}_i^{\rm H}(\mathbf{x})$ is the rate of displacement in the homogenized model and $\dot{u}_i^{\rm H}(0)$ is the rate of displacement at the origin of the macroscopic coordinate system X (the value is described in the macroscopic coordinate system). In this case, we can write

$$\dot{\alpha}_{ij}^{\rm H} = \frac{\partial \dot{u}_i^{\rm H}(\mathbf{x})}{\partial x_j} \tag{7}$$

When we consider the heterogeneity of the microstructure, the rate of real displacement \dot{u}_i^{ε} should be resolved into the rate of homogenized displacement and the rate of perturbed displacement as Eq. (8)

$$\dot{u}_i^\varepsilon = \dot{u}_i^{\rm H}(\mathbf{x}) + \dot{u}_i^{\rm I}(\mathbf{x}) \tag{8}$$

where $\dot{u}_i^1(\mathbf{x})$ is the perturbed term caused by the microscopic heterogeneity. Now, both of these displacements are written in X-coordinate system. Unlike what has been assumed in other research works, $\dot{u}_i^1(\mathbf{x})$ is not the rate of displacement of microstructure. When we consider the order of the scale ratio ε , \dot{u}_i^1 described in the coordinate system X is very small. Therefore, Eq. (8) could be rewritten as Eq. (9) using the coordinate system Y as well as X.

$$\dot{u}_i^\varepsilon = \dot{u}_i^{\rm H}(\mathbf{x}) + \varepsilon \dot{u}_i^{\rm I}(\mathbf{y}) \tag{9}$$

In Eq. (9), the first term $\dot{u}_i^{\rm H}(\mathbf{x})$ is described in the coordinate system X, while the second term $\dot{u}_i^{\rm H}(\mathbf{y})$ is described in the coordinate system Y. By magnifying the microscopic model with the scale ratio ε , it becomes of the same size as the macroscopic model. Still $\dot{u}_i^{\rm I}(\mathbf{y})$ is not the rate of displacement of microstructure.

The rate of displacement of macroscopic model written in the coordinate system X is defined by the

following equation

$$\dot{U}_i^{\text{inacto}}(\mathbf{x}) = \dot{u}_i^{\varepsilon}(\mathbf{x}) \tag{10}$$

By using Eq. (9) and knowing that ε is very small, we can write as follows

$$\dot{U}_i^{macro}(\mathbf{x}) = \dot{u}_i^{\varepsilon}(\mathbf{x}) \cong \dot{u}_i^{\mathrm{H}}(\mathbf{x}) \tag{11}$$

By multiplying both sides of Eq. (5) by $\dot{\alpha}_{ij}^{\text{H}}$ and considering the difference of origins of both coordinate systems X and Y, we obtain the next relation.

$$\dot{\alpha}_{ij}^{\rm H} \left(\mathbf{x}_j - \mathbf{x}_j^{y=0} \right) = \varepsilon \dot{\alpha}_{ij}^{\rm H} y_j \tag{12}$$

where $\mathbf{x}_{j}^{y=0}$ is the position of the origin of the microscopic coordinate system Y written in the macroscopic coordinate system X. When the origin of macroscopic coordinate system is equal to that of microscopic coordinate system, $\mathbf{x}_{j}^{y=0}$ is equal to zero. From the above equations, Eq. (6) can be written in the following way

$$\dot{u}_{i}^{\rm H}(\mathbf{x}) = \varepsilon \dot{\alpha}_{ij}^{\rm H} y_{j} + \dot{\alpha}_{ij}^{\rm H} x_{j}^{y=0} + \dot{u}_{i}^{\rm H}(0)$$
(13)

If we consider only the deformation of the microstructures after the uniform deformation, the rate of displacement of the origin of the microscopic coordinate system Y is zero. Consequently, Eq. (13) yields the next equation

$$\dot{u}_i^{\rm H}(\mathbf{x}) = \varepsilon \dot{\alpha}_{ii}^{\rm H} y_j \tag{14}$$

The rate of displacement of microstructure can be written in the coordinate system Y as

$$\dot{U}_{i}^{\text{micro}}(\mathbf{y}) = \dot{u}_{i}^{\varepsilon}(\mathbf{y}) = \frac{1}{\varepsilon} \dot{u}_{i}^{\varepsilon}(\mathbf{x}) = \frac{1}{\varepsilon} \dot{u}_{i}^{\text{H}}(\mathbf{x}) + \dot{u}_{i}^{1}(\mathbf{y}) = \dot{\alpha}_{ij}^{\text{H}} y_{j} + \dot{u}_{i}^{1}(\mathbf{y}) = \frac{\partial \dot{u}_{i}^{\text{H}}(\mathbf{x})}{\partial X_{j}} y_{j} + \dot{u}_{i}^{1}(\mathbf{y})$$
(15)

The first term of Eq. (15) is the value of coordinates in microscopic coordinate system multiplied by the macroscopic displacement gradient. In summary, the original point of this formulation is the definition of macro- and microscopic displacements as Eqs. (11) and (15), which are used to update the local regions in a macroscopic sense and the microstructures in the numerical analysis.

The rate of Green-Lagrange strains in macro- and microscopic models are defined by Eqs. (16) and (17). To obtain these equations, we used Eqs. (11) and (15), and also the updated Lagrangian formulation. The quadratic term of the strain rate was supposed to be negligible. Eq. (18) denotes the second Piola-Kirchhoff stress in the microstructure. The second Piola-Kirchhoff stress in global structure is defined in the next section.

$$\dot{E}_{ij}^{\text{macro}}(\boldsymbol{x}) = \frac{1}{2} \left(\frac{\partial \dot{U}_{i}^{\text{macro}}(\boldsymbol{x})}{\partial X_{j}} + \frac{\partial \dot{U}_{j}^{\text{macro}}(\boldsymbol{x})}{\partial X_{i}} \right) = \frac{1}{2} \left(\frac{\partial \dot{u}_{i}^{\text{H}}(\boldsymbol{x})}{\partial X_{j}} + \frac{\partial \dot{u}_{j}^{\text{H}}(\boldsymbol{x})}{\partial X_{i}} \right)$$
(16)

N. Takano et al. | International Journal of Solids and Structures 37 (2000) 6517-6535

$$\dot{E}_{ij}^{\text{micro}}(\mathbf{y}) = \frac{1}{2} \left(\frac{\partial \dot{U}_{i}^{\text{micro}}(\mathbf{y})}{\partial Y_{j}} + \frac{\partial \dot{U}_{i}^{\text{micro}}(\mathbf{y})}{\partial Y_{i}} \right) = \frac{1}{2} \left(\frac{\partial}{\partial Y_{j}} (\dot{\alpha}_{ik}^{\text{H}} y_{k}) + \frac{\partial}{\partial Y_{i}} (\dot{\alpha}_{jk}^{\text{H}} y_{k}) + \frac{\partial \dot{u}_{i}^{1}(\mathbf{y})}{\partial Y_{j}} + \frac{\partial \dot{u}_{j}^{1}(\mathbf{y})}{\partial Y_{i}} \right)$$
$$= \frac{1}{2} \left(\frac{\partial \dot{u}_{i}^{\text{H}}(\mathbf{x})}{\partial X_{j}} + \frac{\partial \dot{u}_{j}^{\text{H}}(\mathbf{x})}{\partial X_{i}} + \frac{\partial \dot{u}_{i}^{1}(\mathbf{y})}{\partial Y_{j}} + \frac{\partial \dot{u}_{j}^{1}(\mathbf{y})}{\partial Y_{i}} \right)$$
(17)

$$\dot{S}_{ij}^{\text{micro}}(\mathbf{y}) = C_{ijkl}^{\varepsilon} \dot{E}_{kl}^{\text{micro}}(\mathbf{y})$$
(18)

2.3. Application of the homogenization method to large deformation problem

From Eqs. (4) and (7), we can write the next equation

$$\int_{\Omega} \left(\frac{\partial}{\partial X_{j}} \delta \left(u_{i}^{\mathrm{H}}(\mathbf{x}) + \varepsilon u_{i}^{1}(\mathbf{y}) \right) \right) \left(\frac{\partial}{\partial X_{l}} \left(\dot{u}_{k}^{\mathrm{H}}(\mathbf{x}) + \varepsilon \dot{u}_{k}^{1}(\mathbf{y}) \right) \right) \left(C_{ijkl}^{\varepsilon} + \delta_{ik} S_{jl}^{\varepsilon} \right) d\Omega$$
$$= \int_{\Omega} \delta \left(u_{i}^{\mathrm{H}}(\mathbf{x}) + \varepsilon u_{i}^{1}(\mathbf{y}) \right) \dot{b}_{i} d\Omega + \int_{\Gamma} \delta \left(u_{i}^{\mathrm{H}}(\mathbf{x}) + \varepsilon u_{i}^{1}(\mathbf{y}) \right) \dot{t}_{i} d\Gamma \,\forall \delta u^{\mathrm{H}}(\mathbf{x}), \,\delta u^{1}(\mathbf{y}) \tag{19}$$

where

$$\frac{\partial}{\partial X_l} \left(\dot{u}_k^{\rm H}(\mathbf{x}) + \varepsilon \dot{u}_k^{\rm l}(\mathbf{y}) \right) = \frac{\partial \dot{u}_k^{\rm H}(\mathbf{x})}{\partial X_l} + \varepsilon \frac{\partial \dot{u}_k^{\rm l}(\mathbf{y})}{\partial X_l} = \frac{\partial \dot{u}_k^{\rm H}(\mathbf{x})}{\partial X_l} + \varepsilon \frac{1}{\varepsilon} \frac{\partial \dot{u}_k^{\rm l}(\mathbf{y})}{\partial Y_l} = \frac{\partial \dot{u}_k^{\rm H}(\mathbf{x})}{\partial X_l} + \frac{\partial \dot{u}_k^{\rm l}(\mathbf{y})}{\partial Y_l}$$
(20)

Using the averaging principle by taking the limit of $\varepsilon \rightarrow 0$, Eq. (19) can be separated into two equations, i.e., Eq. (21) for the microstructure and Eq. (22) for the global structure.

$$\int_{\Omega} \frac{1}{|Y|} \int_{Y} \frac{\partial \delta u_{i}^{1}(\mathbf{y})}{\partial Y_{j}} \left(C_{ijkl}^{\varepsilon} + \delta_{ik} S_{jl}^{\varepsilon} \right) \left(\frac{\partial \dot{u}_{k}^{H}(\mathbf{x})}{\partial X_{l}} + \frac{\partial \dot{u}_{k}^{1}(\mathbf{y})}{\partial Y_{l}} \right) dY d\Omega = 0 \quad \forall \delta u^{1}(\mathbf{y})$$

$$(21)$$

$$\int_{\Omega} \frac{1}{|Y|} \int_{Y} \frac{\partial \delta u_{i}^{H}(\mathbf{x})}{\partial X_{j}} \left(C_{ijkl}^{\varepsilon} + \delta_{ik} S_{jl}^{\varepsilon} \right) \left(\frac{\partial \dot{u}_{k}^{H}(\mathbf{x})}{\partial X_{l}} + \frac{\partial \dot{u}_{k}^{I}(\mathbf{y})}{\partial Y_{l}} \right) dY d\Omega = \int_{\Omega} \delta u_{i}^{H}(\mathbf{x}) \dot{b}_{i} d\Omega + \int_{\Gamma} \delta u_{i}^{H}(\mathbf{x}) \dot{t}_{i} d\Gamma$$

$$\forall \delta u^{H}(\mathbf{x})$$

$$(22)$$

Assume the following relation, then the rate of the macroscopic uniform displacement gradient bridges the gap between the macroscopic and microscopic scale.

$$\dot{u}_{i}^{1}(\mathbf{y}) = -\chi_{i}^{kl}(\mathbf{y}) \left(\frac{\partial \dot{u}_{k}^{\mathrm{H}}(\mathbf{x})}{\partial X_{l}} \right)$$
(23)

Then, Eqs. (21) and (22) yield the following solvable equations

$$\int_{Y} \frac{\partial \delta u_{i}^{l}(\mathbf{y})}{\partial Y_{j}} \left(C_{ijmn}^{\varepsilon} + \delta_{im} S_{jn}^{\varepsilon} \right) \frac{\partial \chi_{m}^{kl}(\mathbf{y})}{\partial Y_{n}} \, \mathrm{d}Y = \int_{Y} \frac{\partial \delta u_{i}^{l}(\mathbf{y})}{\partial Y_{j}} \left(C_{ijkl}^{\varepsilon} + \delta_{ik} S_{jl}^{\varepsilon} \right) \, \mathrm{d}Y \quad \forall \delta u^{1}(\mathbf{y})$$
(24)

N. Takano et al. | International Journal of Solids and Structures 37 (2000) 6517-6535

$$\int_{\Omega} \frac{\partial \delta u_{i}^{\mathrm{H}}(\mathbf{x})}{\partial X_{j}} \frac{\partial \dot{u}_{k}^{\mathrm{H}}(\mathbf{x})}{\partial X_{\ell}} \frac{1}{|Y|} \int_{Y} \left\{ \left(C_{ilkl}^{\varepsilon} + \delta_{ik} S_{jl}^{\varepsilon} \right) - \left(C_{ijmn}^{\varepsilon} + \delta_{im} S_{jn}^{\varepsilon} \right) \frac{\partial \chi_{m}^{kl}(\mathbf{y})}{\partial Y_{n}} \right\} dY d\Omega$$
$$= \int_{\Omega} \delta u_{i}^{\mathrm{H}}(\mathbf{x}) \dot{b}_{i} d\Omega + \int_{\Gamma} \delta u_{i}^{\mathrm{H}}(\mathbf{x}) \dot{i}_{i} d\Gamma \quad \forall \delta u^{\mathrm{H}}(\mathbf{x})$$
(25)

 $\chi_m^{kl}(\mathbf{y})$ is the characteristic displacement, which is the solution of microscopic Eq. (24). There are nine modes of characteristic displacements because Eq. (24) tells the asymmetry with respect to k and l. Define the homogenized coefficients as follows

$$C_{ijkl}^{\mathrm{H}} = \frac{1}{|Y|} \int_{Y} \left\{ C_{ijkl}^{\varepsilon} - \frac{\partial \chi_m^{kl}(\mathbf{y})}{\partial Y_n} C_{ijmn}^{\varepsilon} \right\} dY$$
(26)

$$S_{ijkl}^{\rm H} = \frac{1}{|Y|} \int_{Y} \left\{ \delta_{ik} S_{jl}^{\varepsilon} - \frac{\partial \chi_m^{kl}(\mathbf{y})}{\partial Y_n} \delta_{im} S_{jn}^{\varepsilon} \right\} \, \mathrm{d}Y \tag{27}$$

Then, macroscopic equation (25) can be simplified as

$$\int_{\Omega} \frac{\partial \delta u_i^H(\mathbf{x})}{\partial X_j} \Big(C_{ijkl}^H + S_{ijkl}^H \Big) \frac{\partial \dot{u}_k^H(\mathbf{x})}{\partial X_l} \, \mathrm{d}\Omega = \int_{\Omega} \delta u_i^H(\mathbf{x}) \dot{b}_i \, \mathrm{d}\Omega + \int_{\Gamma} \delta u_i^H(\mathbf{x}) \dot{t}_i \, \mathrm{d}\Gamma \quad \forall \delta u^H(\mathbf{x})$$
(28)

By solving Eq. (28), the rate of homogenized displacement $\dot{u}_i^{\rm H}$ can be obtained. Then, the perturbed term $\dot{u}_i^{\rm l}(\mathbf{y})$ is also obtained by Eq. (23). Finally, the rate of microscopic displacement $\dot{U}_i^{\rm micro}(\mathbf{y})$ can be calculated by Eq. (15), which is again the most important equation in our formulation.

The rate of the second Piola–Kirchhoff stress of the global structure is described by Eq. (29). Because the homogenized elastic tensor C_{ijkl}^{H} is not symmetric with respect to k and l, the rate of the second Piola–Kirchhoff stress of the macroscopic model cannot be written in the same form as one of the microscopic model defined by Eq. (18).

$$\dot{S}_{ij}^{\text{macro}}(\boldsymbol{x}) = C_{ijkl}^{\text{H}} \frac{\partial \dot{u}_{k}^{\text{H}}(\boldsymbol{x})}{\partial X_{l}}$$
(29)

3. Discussion on the large deformation of the microstructures

Many composite materials have periodicity of microstructures, such as unidirectional fiber reinforced composites and textile composites including woven and knitted fabric composites. Therefore, the kinematic change of the microstructure of knitted fabric composite material under uni-axial tension at high temperature was investigated experimentally. Tensile tests in course direction, wale direction and 45° off-axis direction were carried out. The microstructure was observed by CCD camera. The dimension of a microscopic unit cell has the order of 1–2 mm. Fig. 2 illustrates the unit cell of knitted fabrics. In this study, knitted fabrics made of aramid fibers and polypropylene were used. Since the used polypropylene is black colored, white marks were written at the cross-points of knitted fabrics so as to trace the large deformation of the microstructures as shown in Fig. 3.

When this composite material was stretched at 443 K, because polypropylene is a thermoplastics and also because knitted architecture allows flexible deformation, both the global structure and microstructure are largely deformed as shown in Fig. 3. The large deformation of the microstructure is

clearly observed particularly in the off-axis tensile test, where the anisotropic principal direction changes during the deformation for some region. This explains the necessity to consider the large deformation of the microstructures.

It is found that the assumption of periodicity holds over the whole structure before deformation. After large deformation (as shown in Fig. 3) in the local region of the whole structure, the periodicity remains and the microstructures are deformed uniformly. More general and practical case is shown in Fig. 4, which is a deep-drawn structure of the same knitted fabric composite material. In this case also we can see the periodicity and the uniform deformation of the microstructures in a local region, except for the corner or edge parts. This experimental fact shows that our assumption which was illustrated in Fig. 1 is valid and that the present homogenization formulation is useful in various practical applications.

If we want to numerically analyze these phenomena by micro-macro modeling, we cannot neglect the change of the homogenized mechanical properties during the deformation, which is caused by the large deformation of the microstructures. Thus, the large deformation problem of the composite materials can be solved only if we can calculate both micro- and macroscopic displacements, update both microstructures and the macrostructure that is an assembly of local regions, and calculate the homogenized properties. The present formulation meets these requirements.

The deformation of the microstructure in one local region is different from that in the other, as shown in Fig. 3. The same is true for the case of deep-draw forming process. In the numerical analysis using the discretized model by finite element method (FEM), we can suppose that the assumption, which is illustrated in Fig. 1 and is validated experimentally, holds in all the finite elements. Therefore, we can solve general large deformation problems by applying the present formulation element by element. Many microstructure models must be considered and calculated in this case, but parallel computing will be effective. For easier and high-speed computing, Takano et al. (1996b, 1998) have proposed a method to use pre-calculated database of homogenized material nonlinearity.

4. Analysis examples

On the basis of the formulation in Section 2, we have developed a computer program to analyze the mechanical behaviors of composite materials under large deformation. The derived P.D.Es are solved



Fig. 2. Unit cell of knitted fabrics.

N. Takano et al. | International Journal of Solids and Structures 37 (2000) 6517-6535



(a) Course direction.



(b) Wale direction.



(c) 45° Off-axis direction.

Fig. 3. Tensile tests of knitted fabric composite material.



Fig. 4. Deep-drawn structure of knitted fabric composite material.



(only fiber bundle)

Fig. 5. Macro- and microscopic modeling by the homogenization method.

with discretization by FEM. Fig. 5 illustrates the macro- and microscopic models by FEM. In the developed program, eight-noded isoparametric hexagonal element is used.

The numerical analysis is carried out as follows. By homogenizing the updated microstructure at each time step, the homogenized mechanical properties are calculated at each step. Then, using the updated homogenized mechanical properties, macroscopic deformation is calculated. That is to say, both the microscopic and macroscopic models are updated in every step.

Two examples are shown below for unidirectional fiber reinforced composite material and knitted fabric composite material. A personal computer was used for these analyses.

4.1. Application to unidirectional fiber reinforced composite material

Fig. 6 shows the finite element model of the unit cell for the unidirectional fiber reinforced plastics. Fig. 6(a) shows the fiber-matrix model, and Fig. 6(b) shows only the fiber model. The mechanical properties of fiber and matrix used in the numerical analysis are shown in Table 1. The fiber and matrix are assumed to be elastic and isotropic. The fiber volume fraction is about 50%.

The analysis of the following three cases are carried out as shown in Fig. 7.

- (I) Tensile deformation in the transverse direction to the fibers
- (II) In-plane shearing deformation on the fibers cross-section
- (III) Out-plane shearing deformation on the fibers cross-section

The results of analyses for the deformation of microscopic structure are shown in Fig. 8 about case (I), Fig. 9 about case (II), and Fig. 10 about case (III). In uniform tensile deformation, only the matrix is deformed but the fiber is hardly deformed. In in-plane shearing deformation, the fiber is rotated without deformation by the macroscopic pure shearing deformation, then the matrix is deformed. In out-plane shearing deformation, the cross-section of the fiber is inclined without deformation and the surface of the microstructure is waved.

4.2. Application to knitted fabric composite material

Suppose a microstructure model of knitted fabric composite material, as shown in Fig. 2, which consists of fiber bundles and matrix. The fiber bundles are to be considered as a homogenized model with anisotropy. Thus, we first calculate the homogenized properties of the fiber bundle using the unit cell model similar to the previous example in Fig. 6. The fiber volume fraction in the bundle is 60% in this case. The mechanical properties used in this calculation is shown are Table 2. The same



Fig. 6. Finite element model of the unit cell of the unidirectional fiber reinforced plastics.

Table	1

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	Fiber	Matrix
Young's modulus (MPa)	71,540	1470
Poisson's ratio	0.3	0.3

polypropylene with Figs. 3 and 4 is taken as matrix, and its Young's modulus is a measured value under 443 K.

The unit cell model of two-layered knitted fabric composite material is shown in Fig. 5. The geometry of this unit cell model coincides with that in our experimental work in Figs. 3 and 4. Numerical analyses were carried out for tensile and shearing deformation. The largely deformed microstructures are shown in Fig. 11. Approximately 30% macroscopic strain was applied. Since both, force and displacement on the boundary of the unit cell are unknown but are solved in the homogenization method using only the periodic condition, the microscopic deformation is very complex, similar to the previous example. As mentioned in the introduction, the definition of the microscopic deformation and the update of the microstructure in the large deformation analysis are highlighted in this paper, but strain and stress are also obtained and considered in the calculation in, for instance, Eq. (27).

The comparison between the numerical analysis and the experimental result is not straightforward because the microscopic deformation is non-uniform even in the uni-axial tensile test as in Fig. 3, while the macroscopically uniform deformation is supposed in the calculation for a small region illustrated in Fig. 1. This also implies that, from the microscopic point of view, the experimentally measured properties of composite materials can sometimes be an averaged value, where various types of microscopic deformation are included. We have to be careful about it, which is known as size-effect.



Fig. 7. Macroscopic boundary conditions.



(a) initial shape



Fig. 8. Tensile defomation in the transverse direction to the fibers.



(a) initial shape



Fig. 9. In-plane shearing deformation on the fibers cross-section.



(a) initial shape



Fig. 10. Out-plane shearing deformation on the fibers cross-section.



Fig. 11. Analyzed large deformation of the microstructure of knitted fabric composite material.

Table 2

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	Fiber	Matrix
Young's modulus (MPa)	71,540	6.86
Poisson's ratio	0.3	0.3

5. Conclusion

For the numerical simulation of the mechanical behaviors of composite materials with periodic microstructure under large deformation, the formulation of the homogenization method applied to large deformation problem was presented. In this formulation, the displacements of both, macroscopic and microscopic model were defined precisely. In the numerical analysis, the microscopic model is updated at each step with microscopic displacement $\dot{U}^{\text{micro}}(\mathbf{y})$ in Eq. (15). By homogenizing the updated microscopic model in every step, the homogenized mechanical properties are calculated. Using them, the macroscopic deformation is calculated.

Discussion on the periodicity of the microstructure after large deformation was described through experimental work for knitted fabric composite material. It was found that the periodicity remains local enough to apply the proposed homogenization formulation to the general composite materials and structures.

Finally, numerical examples were shown for unidirectional fiber reinforced composite material and knitted fabric composite material. In these analyses, however, we did not consider the material nonlinearity of fiber and matrix. Also, only the kinematic change of the knitted architecture (fiber bundles) was considered. The temperature-dependent viscoelastic material model should be used for the matrix for the former problem. For the latter problem, three-scale expansion method must be developed. Moreover, since only one microstructure model is considered in the current examples, more realistic large deformation problems, which are illustrated in Fig. 1 and in Section 3, are expected to be solved.

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