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State-of-the-art of the multi-scale analysis of advanced composite materials by homogenization method

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ABSTRACT

To study numerically the mechanical behaviors of advanced composite materials considering the microscopic phenomena as well as the macroscopic properties and behaviors, a multi-scale modeling and analysis by the mathematical homogenization method with the help of the finite element method(FEM) are reviewed. The hierarchical modeling strategy and the formulation are briefly described first to give some idea of the multi-scale framework. The latter half of this article focuses on the verification of the multi-scale analysis by the homogenization method in its applications to real advanced materials. The first example is the verification of the predicted macroscopic(homogenized) properties based on the microstructure of porous ceramics. In spite of the complexity of the random microstructure, the error between the predicted and the measured values was only 1%. Next, two applications to the process simulation of fiber reinforced polymer matrix composites are presented. The permeability characteristics are evaluated for sheared weave fabrics for resin transfer molding(RTM) simulation, and the thermoforming of FRTP sheet is analyzed considering the large deformation of the knit structure. The largely deformed knit structure during the deep-draw forming was verified by comparison with the experimental results.

1. Introduction

Since various advanced materials including particulate or fiber reinforced composite materials, porous materials and functionally gradient materials have microscopic heterogeneous architecture, the functions or the properties of those materials and components depend strongly on the microstructures. The design and control of the microstructures have been the matter of concern, and will be a key to the future development of the advanced materials. Consequently, there is a growing need for the numerical analysis that can bridge the microstructure and the macroscopic properties, which is recently called multi-scale analysis. The aims of the multi-scale analysis are to predict the macroscopic properties based on the microstructure, to analyze the macroscopic behavior and to analyze the microscopic behavior. The rule of mixture or some other equations such as Halpin-Tsai equation have long been used to predict the macroscopic properties of composite materials. Also, there have been many studies on the so-called micro-mechanics using Eshelby's tensor. However, in the rule of mixture, for instance, only the volume fraction is the parameter that stands for the microscopic architecture. The original micro-mechanics assumes the stress is uniform in the second-phase inclusion. Those assumptions and limitations don't meet the above-mentioned requirements for the multi-scale analysis.

In the computational mechanics field, however, there have been intensive research works during the last decade on the mathematical approach to the multi-scale modeling and analysis of heterogeneous materials. The homogenization method has been the main stream, and therefore this article is devoted to address its advantages and practical applications.

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Section 2 describes the historical review, modeling strategy and formulation of the homogenization method, but the detailed mathematical issues are neglected in this article. Because some people may doubt the validity and the accuracy of such mathematical method when it is applied to real composite materials, section 3 describes the comparison of the predicted macroscopic property with measured one for porous ceramics. Very complex microstructure is modeled semi-automatically and three-dimensionally. As the application to fiber reinforced polymer matrix composites, the prediction of the permeability of resin in plain weave fabrics, which is an important parameter in resin transfer molding (RTM), and the deep-drawing simulation of knit fabric reinforced thermoplastic sheet are shown in section 4. In the latter application, the homogenization method is enhanced to solve large deformation problems, to which other micro-mechanical methods could not be applied. The calculated largely deformed knit structures after deep-draw forming are compared with the experimental results to demonstrate the validity of this method again. The author would like to address the whole story as concisely and easily as possible, and therefore please see the references listed below for the detailed settings in the numerical examples.

2. Multi-scale modeling using homogenization method

In the case of textile composites such as woven or knit fabric reinforced composites, for instance, the hierarchy is now commonly used with the following three scales [1-4]:

micro-scale : fiber
meso-scale : yarn
macro-scale : component or structure

The gap in length between the scales are very large, but the architecture and the behavior at a smaller scale are much influential on the property and the behavior at a larger scale. The aim of the mathematical homogenization method is to describe the behaviors at every scale and the interactive effects between the scales rigorously to the continuum theory of elasticity. It was first developed in the 1970's and early 1980's by applied mathematicians as a mechanical theory of heterogeneous materials[5-7]. In the engineering field, it was applied to the topology design of mechanical components in 1988[8]. Soon after that, its implementation to finite element analysis was in detail presented and some demonstrative examples of fiber reinforced composites were shown [9]. Although the above pioneering studies were for linear elastic problems, the last decade was devoted to enhance it to solve various nonlinear phenomena[10-18]. These studies, which are mainly theoretical ones, include visco-elasto-plastic analysis [10,11], large deformation analysis[12,13], damage propagation analysis[4,14,15], buckling analysis[16], and fluid permeation analysis[17]. The rigorous and consistent description of this theory has led to its enhancement to nonlinear method, which is one of the advantages over other micro-mechanical methods.

In this article, as an introduction to this theory, only the brief description of the formulation for linear elastic problem is given. Please see above references[3-17] for more details. We suppose that the heterogeneous materials such as composite materials consist of periodic microscopic unit cells. Now the periodicity is an assumption, but it may be allowable for textile composites and the case with random microstructure is described in section 3. Define the macroscopic coordinate x and microscopic one $y=x/\varepsilon$ to describe the microscopic behavior, where ε is the scale ratio and is a very small positive number. Based on the two-scale asymptotic expansion method, the displacement can be written as follows:

$$u_i = u_i(x,y) = u_i^0(x) + \varepsilon \; u_i^1\left(x, y=\frac{x}{\varepsilon}\right) \tag{1}$$

where u_i^0 is the macroscopic displacement and u_i^1 is the perturbed term due to the microscopic heterogeneity. u_i^1 is periodic with respect to the microscopic unit cell.

The governing equilibrium equation is written as

$$\int_\Omega E_{ijkl} \frac{\partial u_k}{\partial x_l} \frac{\partial \bar{u}_i}{\partial x_j} d\Omega = \int_{\Gamma_t} t_i \;\; \bar{u}_i \;\; d\Gamma \tag{2}$$

where E_{ijkl} is an elastic tensor and t_i is the traction applied to the boundary Γ_t. If both the macro- and microscopic behaviors are considered, we can't solve Eq. (2) directly. But the mathematical homogenization method enables us to decouple the macro- and microscopic equations that are solvable by conventional finite element method. That is, by substituting Eq. (1) into Eq. (2) and taking the limit of $\varepsilon \to 0$ using the averaging principle, the following microscopic equation that must be satisfied in a microscopic unit cell Y under periodic boundary condition is derived.

$$\int_Y E_{ijpq}\frac{\partial \chi_p^{kl}}{\partial y_q}\frac{\partial \bar{u}_i}{\partial y_j}dY = \int_Y E_{ijkl}\frac{\partial \bar{u}_i}{\partial y_j}dY \tag{3}$$

Here, χ_p^{kl} is so-called the characteristic displacement which relates the microscopic perturbation u_i^1 and the macroscopic strain $\partial u_k^0 / \partial x_l$ as follows:

$$u_i^1 = -\chi_i^{kl}(y)\frac{\partial u_k^0}{\partial x_l} \tag{4}$$

Six modes of characteristic displacements (Kl=11,22,33,23,31, 12) stand for the mismatch of the mechanical properties of the constituents and the geometrical configuration of the constituents with respect to the macroscopic strain field.

The macroscopic equation is also derived as follows:

$$\int_\Omega E_{ijkl}^H \frac{\partial u_k^0}{\partial x_l}\frac{\partial \bar{u}_i}{\partial x_j}d\Omega = \int_{\Gamma_t} t_i \bar{u}_i \, d\Gamma \tag{5}$$

The homogenized elastic tensor E_{ijkl}^H in Eq. (5) is defined by

$$E_{ijkl}^H = \frac{1}{|Y|}\int_Y \left(E_{ijkl} - E_{ijpq}\frac{\partial \chi_p^{kl}}{\partial y_q} \right) dY \tag{6}$$

where $|Y|$ is the volume of the microscopic unit cell. Twenty-one components in the tensor, if needed, can be calculated for arbitrary microstructure architecture.

The sequence of the analysis yields:

STEP 1: Solve the microscopic equation (3) and obtain the characteristic displacement.

STEP 2: Calculate the homogenized elastic tensor by Eq. (6).

STEP 3: Solve the macroscopic equation (5) and obtain the macroscopic displacement.

STEP 4 : Calculate the macroscopic strain and stress.

STEP 5 : Calculate the microscopic stress at a specified point in the macroscopic structure by the following equation:

$$\sigma_{ij} = \left(E_{ijkl} - E_{ijpq}\frac{\partial \chi_p^{kl}}{\partial y_q} \right)\frac{\partial u_k^0}{\partial x_l} \tag{7}$$

Not only the prediction of the macroscopic properties but also the microscopic stress can be evaluated, which is one of the features of this method. Although the above numerical procedure is sequential, theoretically the macro- and microscopic behaviors are studied simultaneously. The derived partial differential equations can be easily solved by finite element method. Actually the left hand sides of Eqs. (3) and (5) yield standard stiffness matrix.

Only the properties of the constituents at the micro-scale, i.e., the fiber and the resin for instance, are necessary for the multi-scale analysis. Fig. 1 shows the example of multi-scale analysis of textile composites [3]. To solve the global behaviors as well as the behaviors of woven yarns and matrix resin, only the properties of fiber and resin are used. In this example, the Hoffman's failure criterion is applied to the yarn at the meso-scale. This just demonstrates the multi-scale framework, but the following sections focus on the verification through applications to real advanced materials.

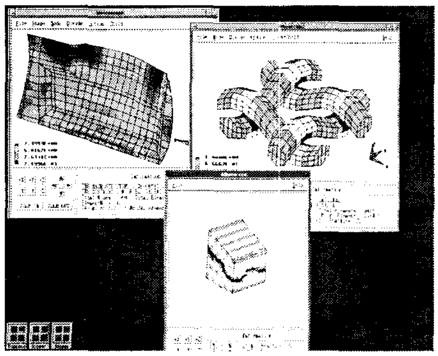


Fig. 1 Example of multi-scale analysis of textile composites.

3. Application to porous ceramics

The multi-scale analysis is based on the microstructure of the material. However, the finite element modeling of the microstructure isn't easy for real heterogeneous materials with random microstructure. To answer to this question, this section describes the prediction of the homogenized properties of porous alumina with needle-like pores, which is compared with the measured values.

The porous alumina is sintered by adding fugitive carbon fibers. The average diameter and length of the needle-like pores are approximately 10mm and 150mm, respectively. The porosity ratio is 3.1%. Because the pores have needle-like

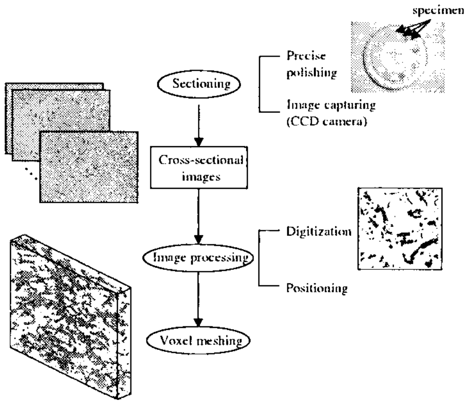


Fig. 2 Schematic of digital image-based modeling for porous alumina.

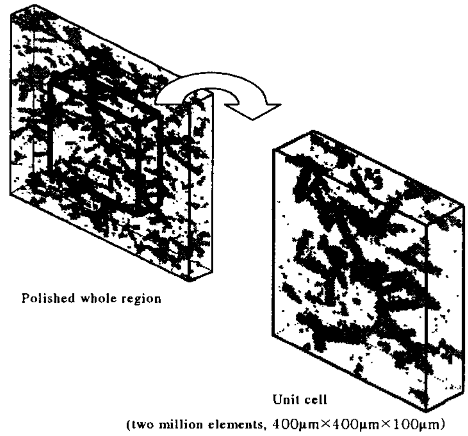


Fig. 3 Unit cell model for homogenization of porous alumina.

shape, three-dimensional modeling is essential. Hence, the digital image-based modeling technique is employed. Its schematic is shown in Fig. 2. The porous alumina is precisely polished by every 2mm in this study, and the cross-sectional view is captured by CCD camera. By repeating this procedure, the three-dimensional microstructure is reconstructed as the voxel image, which is the three-dimensional version of the pixel. The voxel is directly converted into the cubic finite element, which is the voxel element. In this study, the semi-automatically generated voxel element size is equal to the resolution of image, 2mm. See refs. [18-20] for more details.

Although the dispersion of the needle-like pores is random, we can pick up a unit microstructure, to which a periodicity can be applied. Fig. 3 shows one example of choosing a unit cell model. It has been confirmed that choosing this unit cell isn't dependent on the location in the material[20]. The homogenized Young's modulus is calculated by the homogenization method. Note that a standard personal computer is used for this unit cell model with two million elements. The Young's modulus of alumina itself is 404GPa, and the calculated and the measured values of the porous alumina are 362GPa and 366GPa. Some other examples were studied, and the accuracy was very good in all cases. Note that the effectiveness was demonstrated especially for the material with strong anisotropy.

Once the homogenized elastic tensor is obtained, the macroscopic behavior can easily be calculated. Fig. 4 shows an example of four-point bending analysis. The microscopic stress is calculated where maximum macroscopic stress is observed as shown in Fig. 5. Due to the microscopic

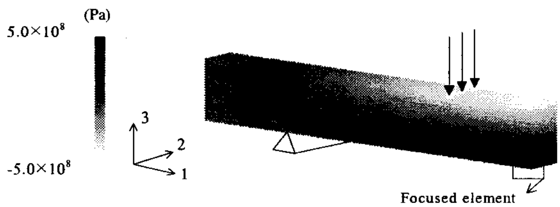


Fig. 4 Macroscopic stress distribution of porous alumina specimen under four-point bending.

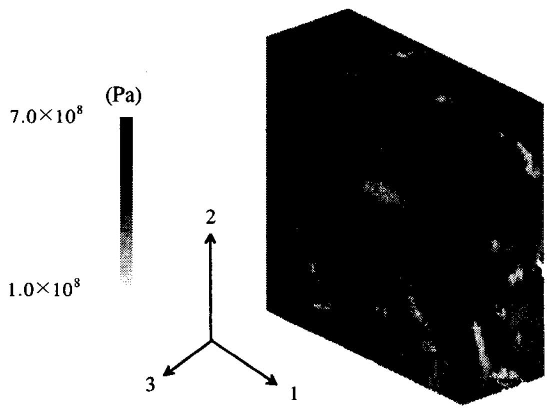


Fig. 5 Microscopic stress distribution in unit cell under four-point bending.

heterogeneity, much higher stress is seen microscopically. The quantitative evaluation of very complex distribution of microscopic stress has been studied in [21]. Fig. 6 shows how stress concentration occurs in the microstructure.

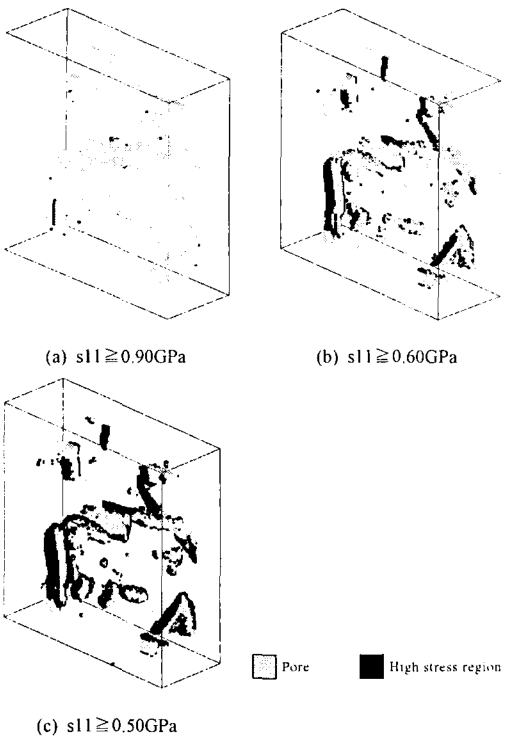
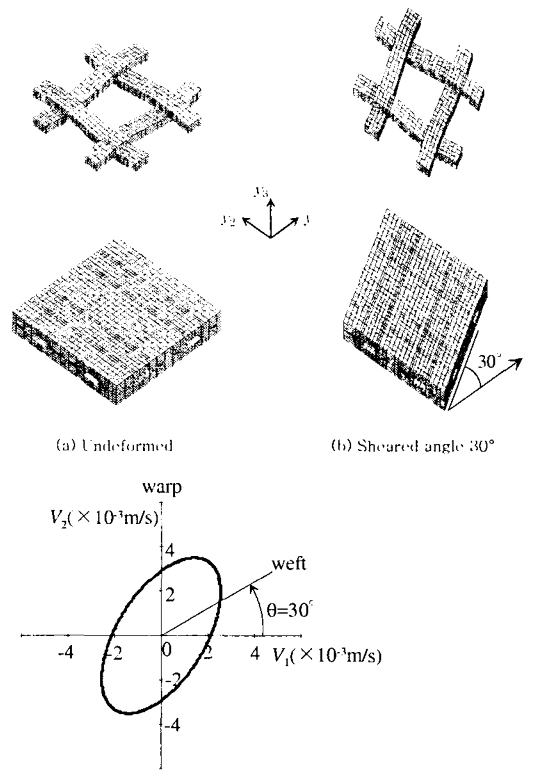


Fig. 6 Stress concentration at micro-scale around pores.



(c) Macroscopic flow front for sheared fabric

Fig. 7 Meso-structure models of plain weave fabrics and calculated macroscopic flow front for sheared fabric.

4. Application to polymer matrix composites

4.1 Prediction of permeability

One of the merits of the homogenization method is that the homogenized properties can be analyzed for arbitrary microstructures and with very good accuracy as was presented in section 3. The application of this method is not limited to solid problems, but this section shows its application to flow problem[17].

The resin transfer molding(RTM) is one of the promising molding methods and we can find many studies on the RTM simulation[22-25]. The permeability, which is a second order tensor, is a key parameter and many efforts were devoted to measure or analyze it[26]. In the analytical approach, the micro- or mesoscopic studies on intra- and inter-tow flows [22,25] and void formation[27,28] and the study on anisotropic permeability tensor[29,30] have been the critical issues. The latter is important because textile performs are sheared in the preforming process. The above problems have not been solved yet, but the homogenization method can provide a breakthrough. Based on the microscopic equilibrium equation, continuity equation and constitutive law for viscous fluid, the Darcy's law can be derived with microscopic equation and characteristic flow function similarly to the formulation in section 2[17,31].

In the author's recent paper[31], the prediction of the permeability is verified first for uni-directional fiber reinforced polymer matrix composites. Then, the demonstrative numerical examples are shown for sheared weave fabrics. Fig. 7 shows the plain weave fabric and sheared fabric models. Note that three-dimensional permeability tensor can be calculated by the three-dimensional model. Fig. 7(c) shows the calculated macroscopic flow front for sheared fabric. In the case of sheared fabric, the non-diagonal term in the permeability tensor is important, which is hardly measured. Quite new results are obtained by the homogenization method such as the microscopic flow field as shown in Fig. 8 and 9. In Fig. 8, the uniform macroscopic pressure gradient is applied

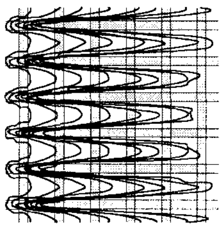
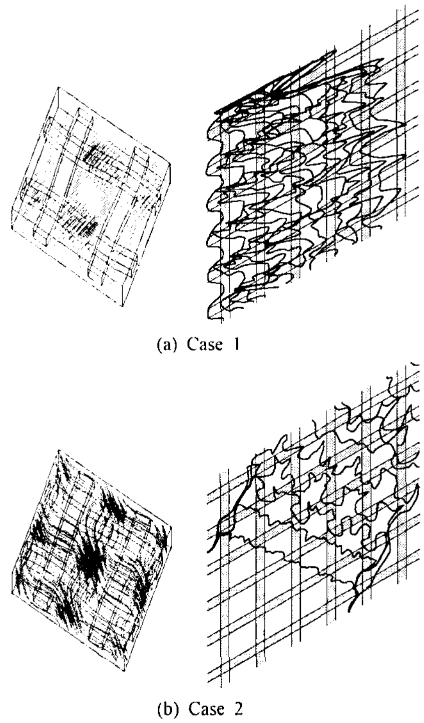


Fig. 8 Mesoscopic flow front for undeformed fabric.



(a) Case 1

(b) Case 2

Fig. 9 Mesoscopic flow front for sheared fabric.

parallel to the yarn, and therefore faster flow is seen between the yarns. However, under the same condition, the microscopic flow is absolutely different for shared fabric as shown in Fig. 9(a). When the macroscopic pressure gradient vector is in the direction of major axis of elliptic macroscopic flow front in Fig. 7, the faster microscopic flow is observed in Fig. 9(b), but still the microscopic flow field is very complex. These kinds of numerical results will lead to the void prediction at the micro- or mesoscale.

4.2 Deep-drawing simulation

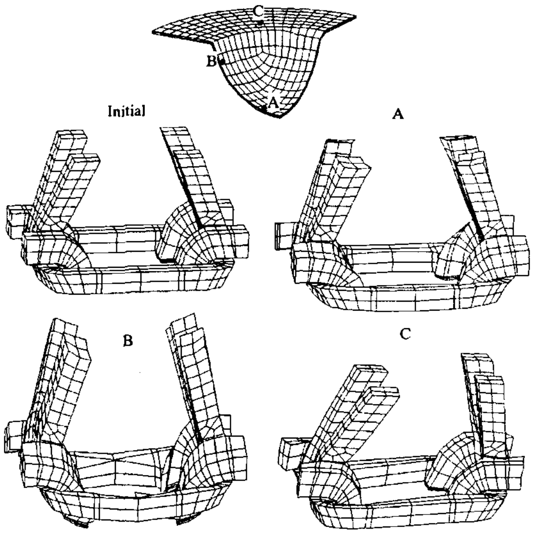


Fig. 10 Largely deformed knit structures (meso-structures) in deep-drawn FRTP sheet.

Above are the linear analyses, but in this section large deformation analysis by the homogenization method is shown. The thermoforming process, which is becoming more and more interested for fiber reinforced thermoplastic sheet [32-35], is analyzed. Differently from the case with thermoplastic sheet without fiber reinforcement[36], the large deformation of the preform during the thermoforming process is very much influential on the properties of the products. The homogenization method can analyze both the macroscopic and microscopic (or mesoscopic) behaviors simultaneously even in the large deformation analysis[13,37]. Fig. 10 shows the numerical results of the deep-drawing analysis of aramid plain knit/polypropylene(PP) composite sheet. Another advantage of the nonlinear homogenization method is that the nonlinear macroscopic properties due to the large deformation of the microstructure (or meso-structure) are calculated without any experimental work. The preform is sheared during the process, which results in the loss of orthotropy of the knit fabric reinforced composites. In this calculation, the microstructure in the yarns is defined as shown in Fig. 11, and only the properties of the aramid fiber and PP are used. The calculated results are compared with the experimental ones. Fig. 12 shows the calculated knit structure at point B in Fig. 10 that is largely stretched. The representative dimensions shown in Fig. 12 coincide very well with the measured results[37]. The validation of the homogenization method is again demonstrated even in the nonlinear analysis.

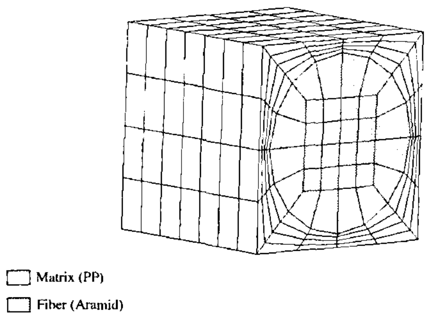


Fig. 11 Microscopic unit cell model in yarns.

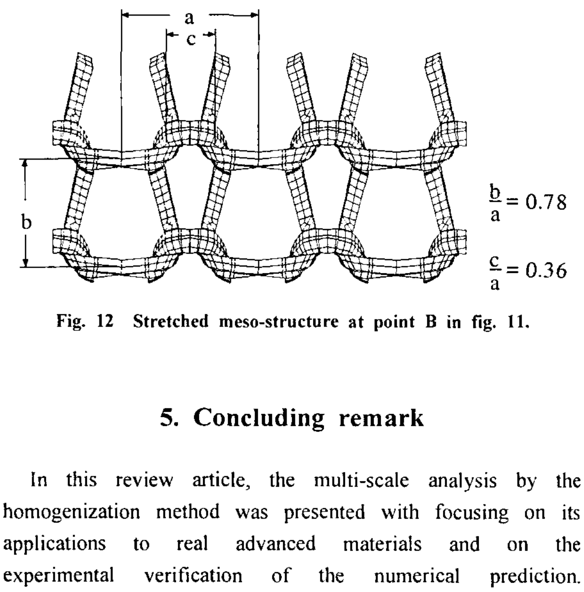


Fig. 12 Stretched meso-structure at point B in fig. 11.

5. Concluding remark

In this review article, the multi-scale analysis by the homogenization method was presented with focusing on its applications to real advanced materials and on the experimental verification of the numerical prediction. Concerning the process simulation of polymer matrix composites, now we can get commercial software such as RTM simulator or thermoforming simulator. The currently existing simulators allow only macroscopic analysis. On the contrary, the microstructure-based simulation presented here can provide us really necessary information because some microscopic parameters must be considered in the design and evaluation of advanced composite materials. Only the microstructure-based method can construct an integrated and consistent RTM simulation including the draping analysis, flow analysis and stress analysis of molded components[31]. Thanks to the pioneering works in the computational mechanics field during the last decade, I hope the multi-scale analysis can be an effective tool for the design and manufacturing of new functional materials.

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