DETERMINATION OF COMPOSITE MATERIAL CONSTANTS BY DIRECT NUMERICAL SIMULATION

Jin Yeon Cho*, Jeong Ho Kim**, Chang Sung Lee and Seung Jo Kim

Department of Aerospace Engineering, Seoul National University
San 56-1, Shillim-Dong, Kwanak-Ku, Seoul 151-742, Korea

SUMMARY: A numerical analysis to predict the elastic material properties of composite structures is accomplished by the Direct Numerical Simulation (DNS) of composite materials and a developed multifrontal code is used. It is paramount in this approach that no artificial assumption for loading or deformation is needed and a highly detailed microstructures of composite structures can be described. In the present analysis, some virtual experiments are executed and the effective elastic moduli of boron/aluminum composites like boron/aluminum are obtained. The results of DNS are compared with the existing theoretical predictions and available experimental data. The validity of basic assumptions applied at theoretical approach are checked and the effects of micro-structures, such as irregular arrangement of fiber on material constants are inspected.

KEYWORDS: mechanical properties, micromechanics, finite element method (FEM), direct numerical simulation (DNS)

INTRODUCTION

Over the years, many efforts and attentions have been given to predict the material constants of fiber-reinforced-composite through the combination of material constants of its constituents. It is physically meaningful since fiber composite is not chemical compound but physical mixture of fiber and matrix. And it is advantageous because the approach can give a rationale for understanding how the stiffness vary according to fiber volume fraction and also a way to acquire the requested stiffness and other material constants. Under this point of view, several mixture models have been proposed for determining material constants of composite.
The classical mixture rule (The modified Voigt-Reuss model[1]) uses the assumptions of uniform fiber direction normal strain ε_{11}, uniform fiber direction normal stress σ_{22}, and uniform shear stress γ_{12}. Among the elastic constants predicted by the rule of mixture, the longitudinal modulus E_1 and Poisson's ratio ν_{12} show good agreement with experiments. Therefore they can be approximated by the simple rule of mixture. However, since neither stress nor strain is uniform in actual composite, models of this type have limitation in predicting accurate material constants. To alleviate the shortcoming, microscopic structures of composite materials have been considered in several studies. The most natural way to understand and predict the effects of microstructures on averaged behaviors of composite may

* Currently at C*enter for Aerospace Research and Education, UCLA, LA, CA 90095-1600*
** Currently at ETRI Supercomputering Center 52 Eoeun-dong Yusong-ku Taejon 305-333 Korea

be direct analysis considering full-scale microscopic model of composite. However, most of the previous works have been carried out through the representative volume element (RVE) called “cell” and/or semi-empirical factors because direct analysis of full-scale microscopic model was nearly impossible so far . And these works using RVE show that the determination of the mechanical properties of a composite lamina depend upon the assumed boundary conditions which need to be applied to the chosen RVE to model different loading conditions[2]. Also the inhomogeneous effects cannot be reflected in RVE. However, at present the situations are being completely changed. In virtue of ever increasing computing power and rapidly advancing computational technologies, it is becoming possible that full-scale microscopic composite models are directly analyzed by finite element method.

Therefore, in this work characterizations of mechanical properties through the direct numerical simulation (DNS) are tackled. By DNS of full-scale microscopic model of composite, highly detail micromechanical behavior inside composite materials according to microscopic structures is observed, and the effects of microstructures, such as irregular arrangement on material constants are inspected.

MICROMECHANICAL ANALYSES OF DETERMING ELASTIC PROPERTIES OF A UNIDIRECTIONAL FIBER COMPOSITE

Micromechanical analyses are based on either the mechanics of materials or the elasticity theory. In the mechanics of materials need some basic assumptions. First of them perfect bonding at the interface is assumed, so that no slip occurs between fiber and matrix materials. The fiber and matrix materials are assumed to be linearly elastic and homogeneous. The matrix is assumed to be isotropic, but the fiber can be either isotropic or orthotropic. Under these assumptions the lamina can be consider to be macroscopically homogeneous, linearly elastic, and orthotropic. These assumptions make it unnecessary to specify the details of the stress and strain distributions at the micromechanical level. Easy-to-use formula, the rule of mixture, can be obtained by this approach. In recent years, thermoviscoplastic properties of the composite materials are obtained by Shin and Kim[3]. Determining elastic moduli of composite material is a difficult problem in elasticity theory. It is first necessary to assume a suitable arrangement of fibers and a geometrical model of the composite lamina and suitable homogeneous boundary conditions are applied to the model. Therefore the elasticity approach often involves numerical solutions of the governing equations because of the complex geometries and boundary conditions.
A third category involves empirical solutions which are based on curve-fitting to elasticity solutions or experimental data. The most widely used semiempirical equations were developed by Halpin and Tsai[4].

The rule of mixture

To describe the elastic properties of composites in terms of constituent properties, the rule of mixture in micromechanics is used. This rule of mixture considers the effect that the Poisson’s ratio difference of fiber and matrix induces force in the fiber direction under transverse loading conditions. The rule of mixture is as follows.

$$E_1 = E_f V_f + E_m V_m \tag{1a}$$

$$\nu_{12} = V_m \nu_m + V_f \nu_f \tag{1b}$$

$$\frac{1}{E_2} = \frac{V_f}{E_f} + \frac{V_m}{E_m} - V_f V_m \frac{V_f^2 E_m / E_f + V_m^2 E_f / E_m - 2 V_f V_m}{V_f E_f + V_m E_m} \tag{1c}$$

$$\frac{1}{G_{12}} = \frac{V_f}{G_f} + \frac{V_m}{G_m} \tag{1d}$$

where V denotes the volume fraction. Subscript f and m denote fiber and matrix respectively and subscript 1 and 2 refer to fiber direction and transverse direction respectively. The Poisson's ratio difference is presented in the third term right-hand side term for E_2.

Elasticity models

The approach using mechanics of materials and the elasticity theory differ substantially in the solution of the resulting boundary value problem. The equations of elasticity must be satisfied at every point in the model, and no simplifying assumptions are made regarding the stress and strain distributions as in the mechanics of materials approach. In view of this difficulty, numerical solutions of the governing equations are often necessary for complex structural geometries. However only the representative volume element RVE is considered rather than full model because it is very difficult to deal with full microscopic model. Adams and Doner[5] used a finite difference solutions to determine the longitudinal shear modulus G_{12} for a rectangular array of fibers. Caruso and Chamis[6] obtained the numerical solution using a "single-cell"(SC) finite element model which was developed from 192 three-dimensional isotropic brick elements. The appropriate constraints on the RVE under various loadings have been determined from symmetry and periodicity conditions lately by Sun and Vaidya[2].
The only existing model that permits exact analytical determination of effective elastic moduli is the Composite Cylinder Assemblage(CCA)[7]. Analysis of the CCA gives closed-form results for the effective properties as follows.

$$E_1 = E_m V_m + E_f V_f + \frac{4(\nu_f - \nu_m)^2 V_m V_f}{V_m / K_f + V_f / K_m + 1/G_m} \tag{2a}$$

$$\nu_{12} = \nu_m V_m + \nu_f V_f + \frac{(\nu_f - \nu_m)(1/K_m - 1/K_f) V_m V_f}{V_m / K_f + V_f / K_m + 1/G_m} \tag{2b}$$

$$G_{12} = G_m + \frac{V_f}{1/(G_f - G_m) + V_m / 2G_m} \tag{2c}$$

Where K is the bulk modulus of material.

VIRTUAL EXPERIMENTS USING DIRECT NUMERICAL SIMULATION

Experimental determination of the composite moduli is difficult, especially when it involves determining the shear modulus. Thus, numerical techniques like finite element method are needed to verify the feasibility of the models. The most of previous numerical methods to estimate composite properties usually involve analysis of a representative volume element (RVE) corresponding to a periodic fiber packing sequence. While the representative volume approaches should be used with semi-

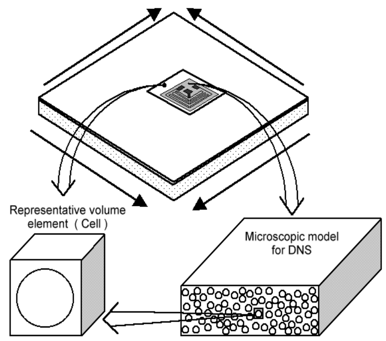
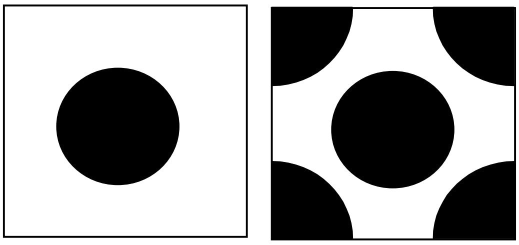


Fig. 1: Description of microscopic model for DNS

empirical factors to consider irregular alignment of fiber and microscopic defect in composite, DNS of full-scale microscopic model can consider those irregular arrangement and microscopic defect directly. In determination of material constants through DNS, any assumptions about local stress or strain conditions are not required, whereas the representative volume element approaches need assumptions about local stress or strain conditions. Let us consider actual pure shear experiment sketched in Fig. 1. Then the only available information is global deformation of which size is similar to the scale of strain gauge. Local loading condition and deformation, of which scale is about representative volume element, are not available. Therefore the approaches using representative volume element should assume local stress or strain condition.

Developed multi-frontal code for DNS



a) Square array *b) Hexagonal array*

Fig. 2 : Representative Volume Element

For direct numerical simulation of composite structures, multifrontal code is developed, where simultaneous equations assembled by FEM is solved by multiple front method[8]. By using the developed multi-frontal code, a virtual experiment is performed.

To obtain the material properties, volume-averaged quantities are introduced as follows.

$$\bar{f} = \frac{1}{V}\int_V f(x,y,z)dV \qquad (3)$$

where V is the total volume of the FEM model. By using this volume-averaged concept, volume-averaged stresses and volume-averaged strains are obtained and elastic moduli can be calculated by the general stress-strain relationship applied to the transversely isotropic materials. Both square array and hexagonal array which are identical with them used by Sun and Vaidya[2] are adopted in this virtual experiment of boron/aluminum composites and shown in Fig. 2. The corresponding constituent properties are given in table 1. In the modeling of composite, 1024 cells are used. The numbers of elements and nodes in square array model are 24,576 and 107,665, respectively. The total degree of freedom differs by the boundary conditions and is larger than three hundred thousand in all cases. 3072 fronts are used in this virtual experiment. The finite element model is shown in Fig. 3.

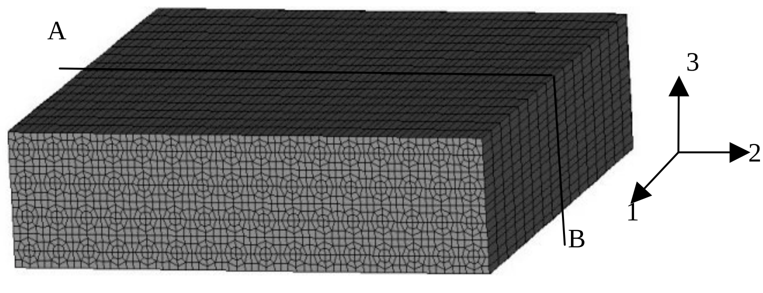


Fig. 3 Finite element model (square array)

	E (GPa)	ν
Boron	379.3 (55.0×10^6 psi)	0.1
Aluminum	68.3 (9.91×10^6 psi)	0.3

Table 1 : Material Properties for boron and aluminum

The numbers of nodes in hexagon array model are slightly larger than that in square array model and are 111,961. The results of DNS under the same volume fraction of 0.47 are presented in table 2. The elastic moduli obtained by DNS are compared the predicted values by the rule of mixture as well as elasticity model(CCM).

Tensile test for longitudinal modulus E_1 and Poisson's ratio v_{12}

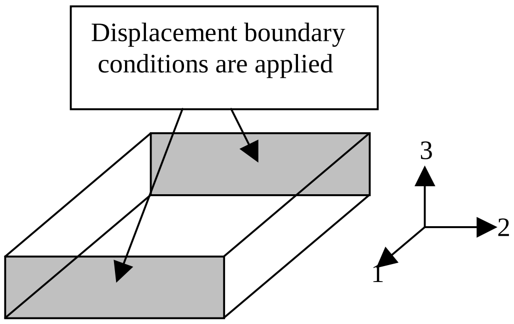


Fig. 4: Boundary conditions for E_1 and v_{12}

A simplified virtual experiment for determining longitudinal modulus E_1 and Poisson's ratio v_{12} is performed by direct numerical simulation in this section. In this test, displacement control is applied . The displacement boundary conditions applied at this simulation are sketched in Fig. 4. In the case of square array, the total degree of freedom is 313,457 and the averaged normal stress $\overline{\sigma}_{11}$ distribution in section-AB is shown in Fig. 5. In Fig. 6, the averaged normal stress $\overline{\sigma}_{11}$ distribution of hexagon array in section-AB is presented and the total degree of freedom of hexagon array is 325,913. The averaged normal strains are constants in section-AB and this agrees well with the basic assumption applied in the rule of mixture.

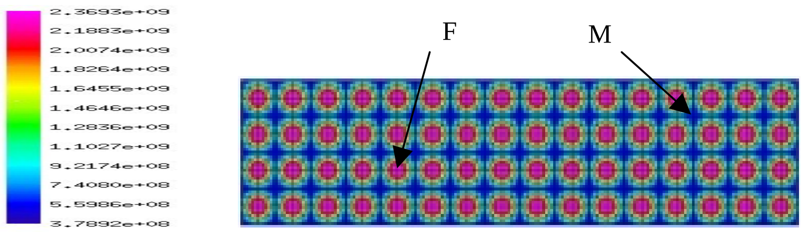


Fig. 5: Contour of the averaged normal stress $\overline{\sigma}_{11}$ in square array

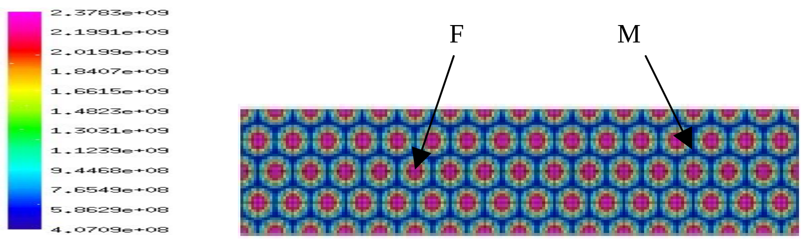


Fig. 6: Contour the averaged normal stress $\overline{\sigma}_{11}$ in hexagon array

As expressed in Fig. 5 and Fig. 6, most of the external loads are maintained by the fibers. Therefore the stress concentration is produced in fiber region F. The averaged normal stress in fiber region F is approximately 6 times larger than that in matrix region M in the both case of square array and hexagon array.

Tensile test for transverse modulus E_2

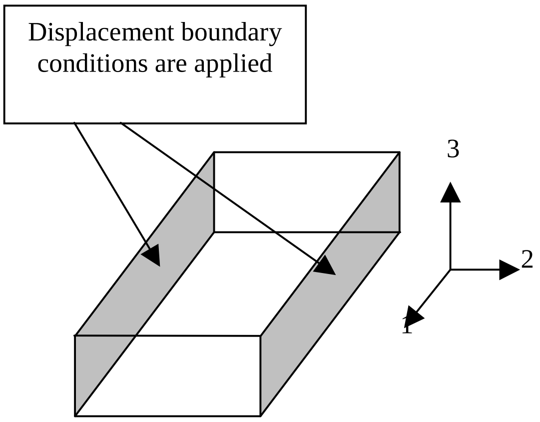


Fig. 7: Boundary conditions for E_2

A numerical experiment for determining transverse modulus E_2 is executed by DNS. The boundary conditions of this case are expressed in Fig. 7. In the case of square array, the total degree of freedom is 321,329 and the averaged normal stress $\bar{\sigma}_{22}$ distribution and the averaged normal strain $\bar{\varepsilon}_{22}$ distribution in section-AB are shown in Fig. 8. In Fig. 9, the averaged normal stress $\bar{\sigma}_{22}$ distribution and the averaged normal strain $\bar{\varepsilon}_{22}$ distribution of hexagon array in section-AB are presented and the total degree of freedom of hexagon array is 333,817.

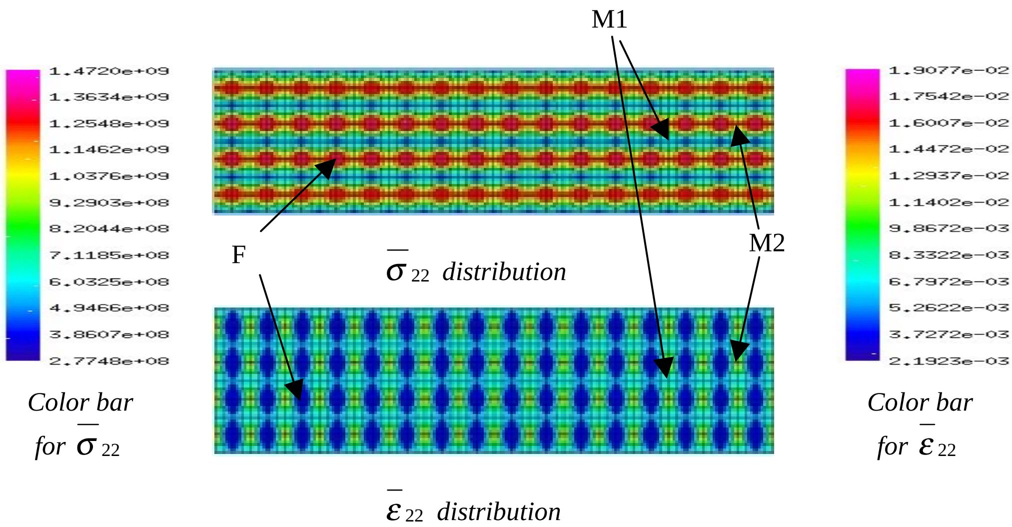


Fig. 8 : Contours of the averaged normal stress $\bar{\sigma}_{22}$ and the averaged normal strain $\bar{\varepsilon}_{22}$ in square array

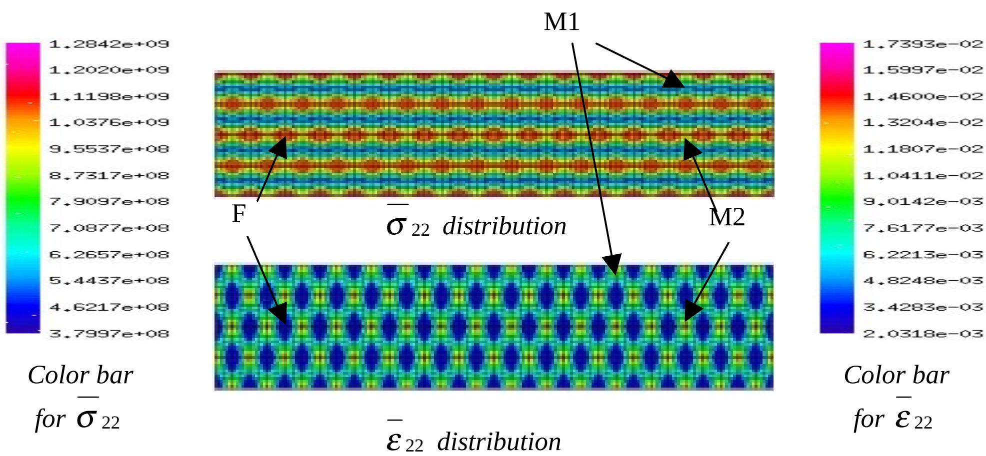


Fig. 9 : Contours of the averaged normal stress $\bar{\sigma}_{22}$ and the averaged normal strain $\bar{\varepsilon}_{22}$ in hexagon array

As shown in Fig. 8 and Fig. 9, the both of the average normal stress $\overline{\sigma}_{22}$ and the average normal strain $\overline{\varepsilon}_{22}$ are distributed differently according to locations. Note that the normal stresses are assumed as the constant value in the rule of mixture. Therefore this assumption is not valid. Especially, the stress concentration occurs at the matrix region between the fibers indicated as M2 in Fig. 8 and Fig. 9. First, let us consider the case of hexagon array. The maximum value of $\overline{\sigma}_{22}$ in region M2 is approximately 3 times larger than the minimum value of $\overline{\sigma}_{22}$ in region M1. The value of $\overline{\varepsilon}_{22}$ is also the maximum value in region M2. The averaged normal strains $\overline{\varepsilon}_{22}$ in the region M2 are roughly 8 times larger than that in the fiber region F. Although region M1 is the matrix region, the stress concentration doesn't occur. In region M1, The value of $\overline{\varepsilon}_{22}$ is larger than the value of $\overline{\varepsilon}_{22}$ in fiber region F but is smaller than the value of $\overline{\varepsilon}_{22}$ in matrix region M2. The distributions of the normal stress and the normal strain of the square array have the same tendency of the hexagon array.

Pure shear test for shear modulus G_{12}

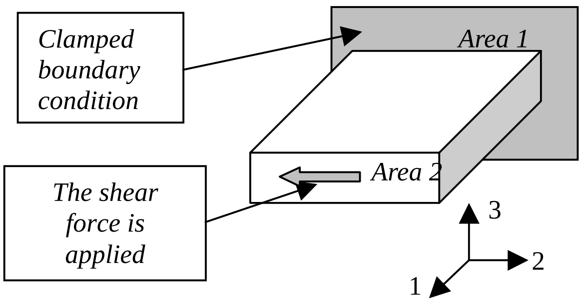


Fig. 10 : Boundary conditions for G_{12}

A similar conditions for pure shear status is imposed through the composite structure model subjected to the uniformly distributed shear load. In Fig. 10, the imposed boundary conditions are expressed. The uniformly distributed shear load is applied at area 2 and the clamped boundary condition is applied at area 1 to guarantee the stability of the numerical solution. In the case of square array, the total degree of freedom is 320,496 and the averaged shear stress $\overline{\sigma}_{12}$ distribution and the averaged shear strain $\overline{\varepsilon}_{12}$ distribution in section-AB are shown in Fig. 11. In Fig. 12, the averaged shear stress $\overline{\sigma}_{12}$ distribution and the averaged shear strain $\overline{\varepsilon}_{12}$ distribution of hexagon array in section-AB are presented and the total degree of freedom of hexagon array is 332,784.

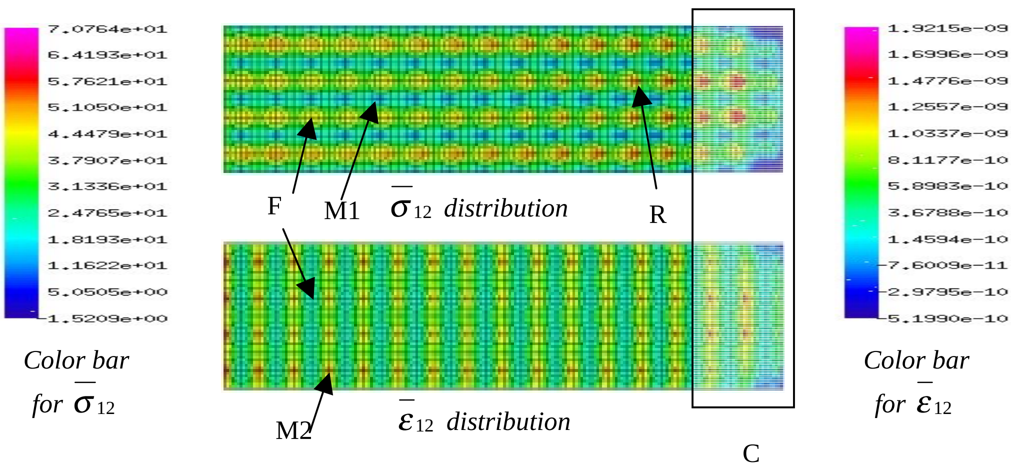


Fig. 11 : Contours of the averaged shear stress $\overline{\sigma}_{12}$ *and the averaged shear strain* $\overline{\varepsilon}_{12}$ *in square array*

As shown in Fig. 11 and Fig. 12, it is observed that the averaged shear stress $\bar{\sigma}_{12}$ and the averaged shear strain $\bar{\varepsilon}_{12}$ in the clamped region C are distributed differently from the other regions of the model. The stress concentration arises highly between the fiber region and the matrix region indicated as R in Fig. 11. In the case of square array, the value of $\bar{\sigma}_{12}$ in region R is no less 11 times larger than the value of $\bar{\sigma}_{12}$ in the matrix region M1. The averaged shear strain $\bar{\varepsilon}_{12}$ in the fiber region F is approximately 40% of that in the matrix region M2.

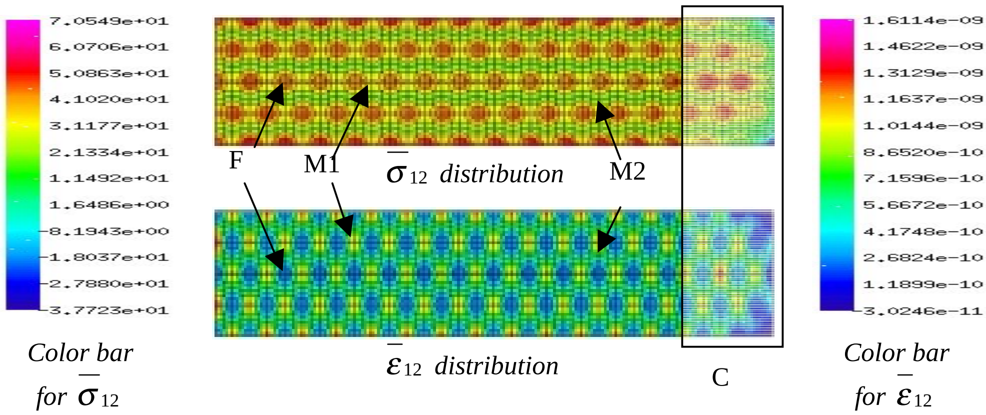


Fig. 12 : Contours of the averaged shear stress $\bar{\sigma}_{12}$ and the averaged shear strain $\bar{\varepsilon}_{12}$ in hexagon array

In the case of hexagon array, the stress concentration is occurred between the fibers indicated as M1 in Fig. 12. The tendency of the averaged shear stress distribution is similar to that in the square array. The values of $\bar{\sigma}_{12}$ in the matrix region M1 and the matrix region M2 are 61% and 23% of that in the fiber region F. In region M1, the averaged shear strain $\bar{\varepsilon}_{12}$ is also very large and is 12 times larger than that in the fiber region F.

Results and discussion

Elastic constants (GPa)	*Square array Ref.[2]*	*Square array Present*	*Hexagonal array Ref. [2]*	*Hexagonal array Present*	*The rule of mixture Eq. (1)*	*Elasticity model CCA, Eq. (2)*	*Experiment Ref. [9]*
E_1	215	215	215	215	214	215	216
E_2	144	143	137	134	130	–	140
ν_{12}	0.19	0.20	0.19	0.20	0.21	0.19	0.29
ν_{23}	0.29	0.25	0.34	0.32	–	–	–
G_{12}	57.2	54.3	54.0	54.0	43.7	54.1	52.0
G_{23}	45.9	46.3	52.5	51.7	–	–	–

Table 2 : Elastic moduli for boron/aluminum composite (V_f =0.47)

In the case of longitudinal modulus E_1, the rule of mixture can predict the molulus exactly. The results obtained by the theoretical approach and the numerical method are the same as that of experiment. This fact is consistent with the validity of the basic assumption that the normal strains are distributed uniformly. Therefore the major Poisson's ratio ν_{12} obtained under the same assumption can be calculated by the simple rule of mixture.

But the results of the other moduli can not be obtained by the simple formula. Through the virtual experiment by DNS, it is verified that these suppositions imposed for E_2 and G_{12} can not be considered to be reasonable. In the case of elasticity approach, shear modulus is predicted more accurately. The results of the numerical approach using the RVE agree well with the results of DNS. This fact indicates that the boundary conditions on the RVE are reasonable.

Inspection on the effect of irregular arrangement

As mentioned before, the numerical method using RVE can not consider the effects of the microstructure but these effects on the material properties can be considered by DNS. To examine the effects of microstructure on elastic modulus, a numerical experiment is executed by DNS where the inhomogeneous model is adopted to simulate the irregular arrngement. In inhomogeneous model, some fiber region is randomly chosen and replaced by matrix. To preserve the volume fraction, the diameter of fiber in inhomogeneous model is increased. Among 64 fibers, 12 fibers are replaced by matrix. The results are shown in table 3.

Elastic constants (GPa)	*Square array (regular)*	*Square array (irregular)*	*Experiment Ref. [9]*
E_1	*215*	*215*	*216*
E_2	*143*	*144*	*140*
G_{12}	*54.3*	*54.7*	*52.0*
G_{23}	*46.3*	*47.0*	–
ν_{12}	*0.20*	*0.19*	*0.29*
ν_{23}	*0.25*	*0.26*	–

Table 3 : Elastic moduli regular & irregular fiber distributrion (V_f =0.47)

As shown in table 3, the elastic moduli are slightly different. The effects of irregular arrangement on the elastic properties can be consider to be insignificant. This is an available information.

Conclusions

In this work, characterization procedure for mechanical properties of composite structures through the direct numerical simulation is proposed. Through numerical experiments by using a developed DNS code, we can obtain the elastic moduli and need no artificial assumption on the stress and strain distribution. And the effects of microstructures, such as irregular arrangement, contiguity of fiber, shape of fiber cross-section, and the defect, on material constants will be examined in detail by DNS. Therefore DNS technique can give many information of composite structures and can be consider as the powerful design tool.

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