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STOCHASTIC MULTISCALE MODELING OF TWO-PHASE MATERIALS BASED ON FIRST-ORDER PERTURBATION METHOD

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ABSTRACT

The homogenization method has been well established in multiscale engineering practise to determine the effective elastic constants of linear elasticity of heterogeneous materials by considering their microstructure. This method was developed to reflect the microscopic structure without looking at details of all of the material points of the body, whenever the mechanical behaviour of the macroscopic body is in question. Nevertheless, in the classical homogenization method, the microscopic characteristics were modelled in deterministic manner. To estimate the expectation and dispersion of macroscopic properties considering uncertainties in microstructure caused by distributing properties of constituent materials, variations in geometry and so on, expensive calculation should be repeated supposedly many times using Monte Carlo simulation. Therefore, this study aims to predict the macroscopic properties of two-phase materials considering uncertainties in microstructure by introducing the stochastic multiscale method. Stochastic finite element method using first-order perturbation-based was combined with homogenization theory to derive the formulation. By assuming the fluctuation arises in microscopic property is distributed in normal distribution, determination of macroscopic properties was formulated in stochastic treatment. Then, the proposed method was established by adding some demonstrative examples that commonly occurred in engineering materials. The numerical results suggest that the uncertainties in microstructure influenced the macroscopic properties of two-phase materials. It indicates the importance of presented stochastic multiscale analysis for microstructure design with considering the microscopic random variations.

Keywords: stochastic multiscale method, perturbation method, heterogeneous materials, macroscopic properties.

INTRODUCTION

Homogenization method has been widely used to predict the macroscopic (homogenized) of heterogeneous materials in multiscale engineering problem, especially when the microstructure was considered [1,2]. This approach enables the simplification of discretization process without looking into details of each point of microstructure and at the same time, the computational time can be reduced.

However, in classical homogenization theory, the macroscopic response has been obtained in deterministic manner. Since the randomness exists in the microstructure, the multiscale analysis should be treated in stochastic nature. To consider random variations of microstructure caused by distributing properties of constituent materials, fluctuation of geometry and so on, the use of conventional approach of Monte Carlo simulation will require huge computational time. Only a few computational schemes are available for evaluation of random media in stochastic manner. Recently, stochastic FEM was combined with homogenization theory using perturbation-based [3,4] and spectral methods [5,6] to calculate the macroscopic response due to local behaviors in microstructure such as in trabecular bones [7,8] and cellular materials [9]. But these studies are only considered one random variable each time to estimate the stochastic response.

Therefore, this paper proposed the formulation of stochastic homogenization method applied to two-phase materials to calculate the variation of macroscopic homogenized properties. First, the theoretical framework of stochastic homogenization using first order perturbation method was derived. Then, the applicability of the computational formulation was tested on demonstrative examples of two-phase materials; (1) fiber reinforced composite and (2) honeycomb microstructure.

FRAMEWORK OF STOCHASTIC HOMOGENIZATION PERTURBATION-BASED

Consider a unit cell representing an inhomogeneous solid with periodically arranged microstructure and containing various types of random microstructures such as fibers, particles, polycrystallite or porous materials as shown in Figure 1. If this unit cell has a periodic microstructure, the effective elastic properties or homogenized properties of represented structure can be obtained using classical homogenization theory. But because of the random nature in microstructure, the homogenized properties D^H could be influenced by the uncertain parameters such as the morphology of microstructure *A*, material types *M* and volume fraction *V*, as variables of geometrical information *X*, and mechanical properties of constituents *D*. This relationship can be summarized as in eq. (1)

$$D^H = f\left(\left(M_k, V_k, A_k\right), D_k\right) \tag{1}$$

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where k is the number of constituent materials and f denotes the function of D^H .

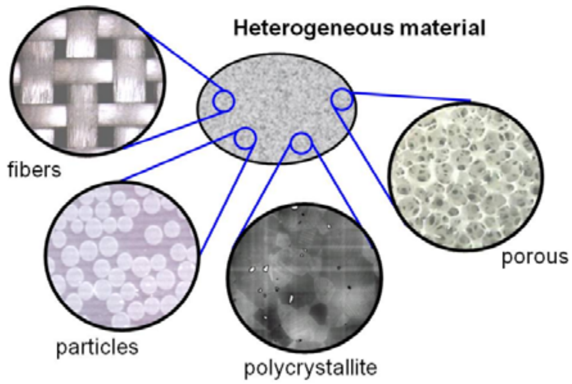

Figure-1. Microstructure of heterogeneous materials.

In this paper, however, we assumed only the mechanical (microscopic) properties of constituent D have a small random fluctuation. Then, the microscopic property is written as a sum of deterministic term D^0 and stochastic one that denotes by α.

$$D_k = D_k^0(1+\alpha_k) \tag{2}$$

Next, by taking into account this fluctuation, the homogenized property is formulated as a function of α. If this function is approximated in expansion form, then the approximation of homogenized property is written as,

$$D_k^H = D_k^H(\alpha_k) \approx \sum_m \left(D^H\right)^m \phi^m \tag{3}$$

where ϕ is a fluctuation with m-th order. Based on perturbation theory, ϕ in above equation is equal to α. Then, the homogenized property is written in perturbation form as eq. (4).

$$D_k^H = \left(D_k^H\right)^0 + \left(D_k^H\right)^1 \alpha_k + \left(D_k^H\right)^2 \alpha_k^2 + \ldots \tag{4}$$

Considering the fluctuation of α was characterized by probability density function f (α), an expectation of the homogenized elastic tensor can be calculated as follows.

$$\begin{aligned}\mathrm{Exp}\left(D^H\right) &= \int_{-\infty}^{\infty} D_k^H(\alpha_k) f(\alpha_k) d\alpha_k \\ &\approx \int_{-\infty}^{\infty} \left\{\left(D_k^H\right)^0 + \left(D_k^H\right)^1 \alpha_k + \cdots\right\} f(\alpha_k) d\alpha_k\end{aligned} \tag{5}$$

Applying the first-order perturbation method to this calculation and assuming the stochastic variable α is distributed in normal distribution, the expected value and variance of the homogenized property is computed in equation (6) and (7), respectively.

$$\mathrm{Exp}\left(D^H\right) = \left(D_k^H\right)^0 \tag{6}$$

$$\begin{aligned}\mathrm{Var}\left(D^H\right) &= \int_{-\infty}^{\infty} \left(D_k^H(\alpha_k) - \mathrm{Exp}\left(D^H\right)\right)^2 f(\alpha_k) d\alpha_k \\ &= \left(D_k^H\right)^1 \left(D_k^H\right)^1 \int_{-\infty}^{\infty} \alpha_k{}^2 f(\alpha_k) d\alpha_k \\ &= \left(D_k^H\right)^1 \left(D_k^H\right)^1 \mathrm{cov}[\alpha_k, \alpha_k]\end{aligned} \tag{7}$$

Next, zero-th and first order of the stochastic homogenized property should be derived in order to solve equation (6) and (7).

DISCRETIZATION OF STOCHASTIC FINITE ELEMENT AND HOMOGENIZATION PROCEDURE

Based on deterministic homogenization theory, the geometrical information **X** in eq. (1) is replaced by the characteristic displacement χ, and written as,

$$D^H = F(\chi(M_k, V_k, A_k), D_k) = \frac{1}{|Y|}\int_Y D_k \left(I - \frac{\partial \chi}{\partial y_k}\right) dY \tag{8}$$

where $|Y|$ is the volume of the unit cell Y. Then, this equation is discretized by finite element methods as,

$$D_k^H = \frac{1}{|Y|}\int_Y D_k \, dY - \frac{1}{|Y|}\int_Y D_k B_y \chi_k \, dY \tag{9}$$

χ in eq. (9) is the solution of microscopic equation in the following linear algebraic equation form.

$$\begin{aligned}K_k \chi_{kl}^{pq} &= F^{pq} \\ \int_Y B^T D_k B \, dY \left(\chi_{kl}^{pq}\right) &= \int_Y B D_{kl}^{pq} dY\end{aligned} \tag{10}$$

Since the random fluctuation arises in microscopic property D, then the stiffness matrix K and vector F are approximated using first-order perturbation [10].

$$\begin{aligned}K_k &\approx K_k^0 + K_k^1 \alpha_k \\ &= \int_Y B^T D_k^0 B dY + \left\{\int_Y B^T \left.\frac{\partial D_k}{\partial \alpha_k}\right|_{\alpha=0} B dY\right\}\alpha_k\end{aligned} \tag{11}$$

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$$F_k^{pq} \approx \left(F_k^{pq}\right)^0 + \left(F_k^{pq}\right)^1 \alpha$$
$$= \int_Y B\left(D_k^{pq}\right)^0 dY + \left\{ \int_Y B \frac{\partial \left(D_k^{pq}\right)^0}{\partial \alpha_k}\bigg|_{\alpha=0} dY \right\} \alpha_k \tag{12}$$

The order of '0' shows the deterministic term, whilst '1' corresponds to the first-order differential for stochastic variation α_k at $\alpha_k = 0$. When the random quantities are inserted in K and F of equation (10), the linear algebraic equation should be rewritten. Hence, χ is also expressed in an approximation form.

$$\chi_k^{pq} \approx \left(\chi_k^{pq}\right)^0 + \left(\chi_k^{pq}\right)^1 \alpha_k \tag{13}$$

Substitute equations (11-13) into linear algebraic equation will give the following equation.

$$\left[K_k^0 + K_k^1 \alpha_k\right]\left\{\left(\chi_k^{pq}\right)^0 + \left(\chi_k^{pq}\right)^1 \alpha_k\right\} = \left\{\left(F_k^{pq}\right)^0 + \left(F_k^{pq}\right)^1 \alpha_k\right\} \tag{14}$$

By equating the order of α in equation (14), the solution of zero-th and first-order of χ is calculated as,

$$\left(\chi_k^{pq}\right)^0 = \left[K_k^0\right]^{-1}\left(F_k^{pq}\right)^0 \tag{15}$$

and

$$\left(\chi_k^{pq}\right)^1 = \left[K_k^0\right]^{-1}\left\{\left(F_k^{pq}\right)^1 - K_k^1\left(\chi_k^{pq}\right)^0\right\} \tag{16}$$

Finally, the zero-th and first-order of stochastic variation of the homogenized properties can be calculated by equating the order of α, as written in equation (18) and (19) respectively.

$$\left(D_k^H\right)^0 = \frac{1}{|Y|}\int_Y D_k^0\, dY - \frac{1}{|Y|}\int_Y D_k^0 B_y \chi_k^0\, dY \tag{18}$$

$$\left(D_k^H\right)^1 = \frac{1}{|Y|}\int_Y D_k^1\, dY - \frac{1}{|Y|}\int_Y \left(D_k^0 B_y \chi_k^1 + D_k^1 B_y \chi_k^0\right) dY \tag{19}$$

NUMERICAL ANALYSES OF TWO-PHASE MATERIALS

Two sets of numerical simulations are presented to illustrate the applicability of the present stochastic homogenization method for the analysis of dispersion of homogenized properties in two-phase heterogeneous materials. All numerical analyses in this section are performed using 3D voxel elements.

Fiber-reinforced composite

Figure-2 shows the finite element model of unit cell for fiber reinforced composite as a periodic microstructure. Volume fraction of fiber in this example is 0.25. Microscopic properties of the constituents are listed in Table-1. In this example, the fluctuation of microscopic property (D) that has been derived in the previous chapter is assumed arise in Young's modulus, E. Considering the random variation in Young's modulus, hence the stochastic approximation of E can be written as follows.

$$E_k = E_k^0\left(1 + \alpha_k\right) \tag{20}$$

By assuming the fluctuation of random variable is distributed in Gaussian normal distribution and referring to the input value in Table-1, the Young's modulus of E-glass fiber was set as 72.4 GPa with standard deviation of 3.982 GPa, whilst epoxy resin (matrix) was set as 2.75 GPa with standard deviation of 0.0413 GPa. Noted here that the stochastic variables value have been set-up based on recommendation in literature with small coefficient of variance [4]. Poison's ratios for both constituents were set as deterministic variable.

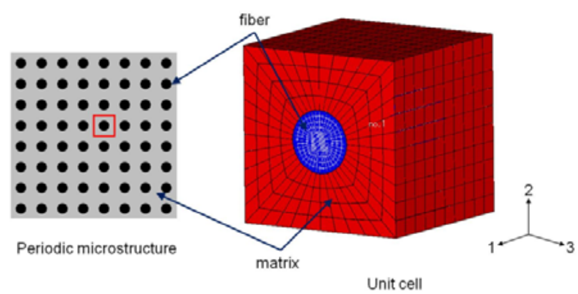

Figure-2. Unit cell of fiber reinforced composite (FRC).

Table-1. Microscopic properties of constituents of FRC.

	E-Glass (fiber)	**Epoxy** (matrix)
Young's modulus, E (GPa)	72.4	2.75
Poison's ratio, ν	0.2	0.35
Standard deviation of stohastic variable, σ_α	0.055	0.015

Honeycomb microstructure

In the second example, the same problem set-up as in the first example was used to determine the stochastic homogenized properties of two-phase

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honeycomb microstructure. Figure-3 shows the finite element model of honeycomb that consists of 5052 aluminum and adhesive materials. Considering the honeycomb as periodic microstructure, the unit cell is selected to represents the homogenized properties. Table-2 listed the microscopic properties of the constituent materials. Young's modulus for aluminum in this example is 70 GPa with standard deviation of 3.85 GPa, whilst for adhesive is set as 2.2 GPa with standard deviation 0.033 GPa.

RESULTS AND DISCUSSIONS

The calculated expected value of homogenized properties for fiber reinforced composite is written in the matrix form as follows.

$$\mathrm{Exp}(\mathbf{D^H})=\begin{bmatrix} 11.4264 & 2.5472 & 2.5472 & 0 & 0 & 0 \\ & 5.0705 & 2.6220 & 0 & 0 & 0 \\ & & 5.0705 & 0 & 0 & 0 \\ & & & 1.1871 & 0 & 0 \\ & & & & 1.2325 & 0 \\ & sym & & & & 1.2325 \end{bmatrix} \text{(GPa)}$$

Obviously, the result shown that the homogenized properties were transverse-isotropic with the highest stiffness was found at axis-1. Since the present formulation using first order perturbation, the expected value for both cases (fiber and matrix variations) was same. Considering the fluctuation of Young's modulus in fiber, the variance of homogenized properties is obtained as follows.

$$\mathrm{Var}(\mathbf{D}^{\mathbf{H}}_{\alpha_{\mathbf{fiber}}})=\begin{bmatrix} 160.0420 & 0.0024 & 0.0024 & 0 & 0 & 0 \\ & 0.0115 & 0.0030 & 0 & 0 & 0 \\ & & 0.0115 & 0 & 0 & 0 \\ & & & 0.0003 & 0 & 0 \\ & & & & 0.0008 & 0 \\ & sym & & & & 0.0008 \end{bmatrix} \text{(MPa)}$$

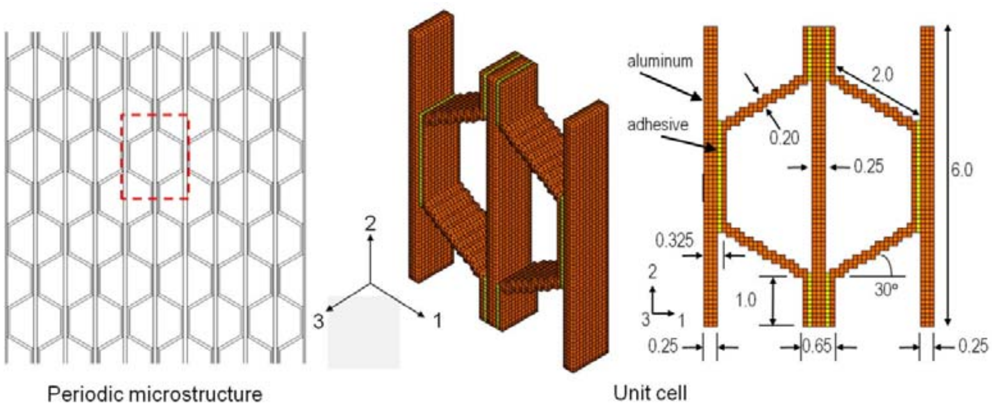

Figure-3. Periodic microstructure of honeycomb (dimension in mm).

Table-2. Microscopic properties of constituents of honeycomb sandwich plate.

	5052 aluminium	Adhesive epoxy
Young's modulus, *E* (GPa)	70	2.2
Poison's ratio, ν	0.3	0.35
Standard deviation of stohastic variable, σ_α	0.055	0.015

Whereas the variance of homogenized properties due to matrix variation is written as follows.

$$\mathrm{Var}(\mathbf{D}^{\mathbf{H}}_{\alpha_{\mathbf{matrix}}})=\begin{bmatrix} 3.8801 & 1.4278 & 1.4278 & 0 & 0 & 0 \\ & 5.6450 & 1.5101 & 0 & 0 & 0 \\ & & 5.6450 & 0 & 0 & 0 \\ & & & 0.3116 & 0 & 0 \\ & & & & 0.3329 & 0 \\ & sym & & & & 0.3329 \end{bmatrix} \text{(MPa)}$$

The results suggest that the fiber variation in microscopic property gives the highest variance of homogenized properties in axis-1, whereas the matrix variation produces the highest variance of homogenized properties in axes-2 and 3. Hence, the fluctuation of microscopic property in fiber reinforced composite influenced to the variation behavior of homogenized properties but the material characteristic as transverse-isotropic is still remain. Next, the expected value of homogenized properties for honeycomb microstructure was obtained below.

$$\mathrm{Exp}(\mathbf{D^H})=\begin{bmatrix} 1.5426 & 1.0832 & 0.7976 & 0 & 0 & 0 \\ & 15.0524 & 4.8497 & 0 & 0 & 0 \\ & & 19.8111 & 0 & 0 & 0 \\ & & & 5.8703 & 0 & 0 \\ & & & & 1.0012 & 0 \\ & sym & & & & 0.1297 \end{bmatrix} \text{(GPa)}$$

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Similar to the first example, the highest stiffness was found in axis-3. It proves that highest stiffness is always in the elongated direction of periodic microstructure. The variance of homogenized properties for both aluminum and adhesive variations are shown in the following.

$$\mathrm{Var}(\mathbf{D}^{\mathbf{H}}_{\alpha_{\text{aluminum}}})=\begin{bmatrix} 2.3370 & 1.8182 & 0.7608 & 0 & 0 & 0 \\ & 642.5880 & 64.2741 & 0 & 0 & 0 \\ & & 1160.2160 & 0 & 0 & 0 \\ & & & 103.4221 & 0 & 0 \\ & & & & 1.4288 & 0 \\ sym & & & & & 0.0346 \end{bmatrix} \text{(MPa)}$$

$$\mathrm{Var}(\mathbf{D}^{\mathbf{H}}_{\alpha_{\text{adhesive}}})=\begin{bmatrix} 0.0991 & 0.0213 & 0.0197 & 0 & 0 & 0 \\ & 0.0513 & 0.0130 & 0 & 0 & 0 \\ & & 0.0116 & 0 & 0 & 0 \\ & & & 0.0001 & 0 & 0 \\ & & & & 0.0222 & 0 \\ sym & & & & & 0.0001 \end{bmatrix} \text{(MPa)}$$

The highest variance for aluminum variation was found at axis-3, whilst the highest variance due to adhesive variation was obtained at axis-1. These results showed that other than microscopic property, the geometry also contribute to the variation of homogenized properties. Hence, the present study has successfully predicted the homogenized properties of two-phase materials in stochastic manner and proves the significance of considering random variation in microstructure in order to estimate accurate stochastic homogenized properties especially for microstructure design and fabrication purpose.

CONCLUSIONS

In the present study, random variations in microscopic property for two-phase materials was considered in the mathematic model to obtain the expected value and variance of homogenized properties using a stochastic homogenization method based on first-order perturbation approach. The numerical results showed the small fluctuation that arise in microscopic property have a significance effect to the stochastic homogenized properties of fiber reinforced composite and honeycomb microstructure. This finding indicates the importance of stochastic multiscale analysis for design and fabrication of two-phase materials in order to obtain a precise macroscopic property variation.

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