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3D stochastic computational homogenization model for carbon fiber reinforced CNT/epoxy composites with spatially random properties

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ABSTRACT

In this paper, a 3D stochastic computational homogenization model for carbon fiber-reinforced (CFR) CNT/epoxy matrix composites was presented. Stochastic waviness, agglomeration and orientation of CNT fillers cause random spatial variations of the elasticity tensor of the CNT/epoxy matrix within a microscale RVE, resulting in probabilistic variations of the effective homogenized stiffness of the RVE. The present computational homogenization model is based on two-scale asymptotic homogenization theory. An ensemble average of the multiple homogenized effective stiffnesses was obtained for structural analysis of the macroscale CFR CNT/epoxy composite materials. From the proposed model, we could observe significant effects of the CNT alignment orientations, agglomeration and waviness on the effective stiffnesses. Effective stiffness changes of a microscale RVE caused by the nanoscale uncertainties were investigated. The proposed multiscale modeling method and approach will be a basis for hierarchical multiscale material design of nanocomposite materials.

1. Introduction

Nanofillers such as graphene and carbon nanotubes (CNT) can greatly enhance thermomechanical and electrical properties of many advanced composites for aerospace applications [1]. For example, CNT-reinforced epoxy (CNT/epoxy) are used to enhance stiffness, strength [2,3], fracture toughness [4], impact resistance [5,6], reduction of creep deformation [7], lightning strike resistance [8] and damping characteristics [9] of carbon fiber-reinforced plastic composite materials. Despite superior physical properties of single pristine CNT, it is challenging to scale up such advantages to the macroscale materials because of large variabilities of the waviness and agglomeration of CNT bundles [10–12]. The CNT/epoxy nanocomposites hold spatial variations of properties caused by the alignment orientation, agglomeration and waviness. Therefore, we should take into account spatial randomness of CNT/epoxy nanocomposites.

To obtain effective stiffness properties of a representative volume element (RVE), various analytical approaches are available, for example, Mori-Tanaka [13], Self-consistent method [14,15], Eshelby equivalent inclusion method [16], differential scheme [17], etc. These analytical or semi-analytical methods can predict effective properties of composite materials having spherical, elliptical, or cylindrical inclusions. Asymptotic analysis method for periodic microstructures [18,19] is the basis of the multiscale computational homogenization method which is versatile and practical for homogenization of heterogeneous composite materials like CNT/epoxy nanocomposites. We could find a plethora of literature devoted to computational homogenization methods [20–31] and multiscale analysis studies [32–37].

Homogenization of random microstructures with varying volume fraction, stiffness contrast, shape, orientation, or porosity etc. has been studied for different material systems by many others [38–44]. Recently, Savvas et al. utilized a homogenization scheme [31] in order to assess effects of material and geometric uncertainties on the effective properties [42]. Xu et al. presented mathematically formulated stochastic homogenization model to simulate variability of the global effective stiffness based on a concept of the stochastic representative volume element (SRVE) [43]. Song et al. proposed RVE models having 3D straight CNT network in the polymer matrix [45] focusing on the percolation threshold for electric conductivity of CNT nanocomposites. Most of existing stochastic homogenization studies for composite materials assumed material uncertainties as random variables whereas few research handled as spatial random fields for only two-dimensional case [46,47] and performed random realizations via Monte Carlo simulations. Further study on the 3D two-scale computational asymptotic homogenization method for nanocomposites with spatial material randomness is still on demand.

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In this paper, we proposed a 3D FE-based computational asymptotic homogenization model for CFR CNT/epoxy composite materials. In Section 2, methods of modeling 3D random fields and CNT/epoxy materials based on micromechanics are delineated. In Section 3, we proposed a 3D computational homogenization model for CFR CNT/epoxy composite materials and kinematic periodic boundary conditions (PBC) on non-matching FE meshes were presented. Section 4 includes numerical simulation results and discussions to investigate effects of CNT uncertainties on macroscale material properties. Finally, conclusions were made in Section 5.

2. Modeling of CNT-reinforced epoxy with material uncertainties

Wavy CNT fillers are dispersed in the epoxy resin with random agglomerations and orientations. Waviness of CNT fillers is also an important factor that determines mechanical properties of CNT nanocomposites. New CNT/epoxy modeling features of the proposed model are illustrated in Fig. 1. In the modeling of the CNT/epoxy, we take the agglomeration, orientation and waviness as spatially varying random fields. Such properties are random in the matrix region of the microscale RVE. Orientation, local volume fraction and waviness at two arbitrary points, p and q are correlated with specified covariance functions.

2.1. Three-dimensional random field discretization by Karhunen-Loève expansion

Let us consider an upper scale spatial domain Ω. Boldface variables in all equations represent matrix or vector. The infinite dimension of 3D random fields in the probability space is reduced to finite dimensions by three-dimensional Karhunen-Loeve expansion (KLE) method. The KLE decomposes a spatial random field $H(\vec{\boldsymbol{x}})$ to a deterministic and a stochastic part as follows

$$H(\vec{\boldsymbol{x}}) = < H(\vec{\boldsymbol{x}}) > + \sum_{i=1}^{m} \sqrt{\lambda_i}\phi_i(\vec{\boldsymbol{x}})[\xi_i],\ \vec{\boldsymbol{x}} \in \Omega \tag{1}$$

where $<H(\vec{\boldsymbol{x}})>$ is the mean value; ξ_i is the normal variable; λ_i, $\phi_i$are the eigenvalue and eigenfunction of an analytical covariance kernel, respectively; [·] means that ξ_i is a set of sampled normal variables; $\vec{\boldsymbol{x}}$ is the position vector in the spatial domain Ω; and m is the truncation order of KLE series. The random fields are assumed to be ergodic random process for the sake of simplicity. Therefore, the spatial mean value $<H(\vec{\boldsymbol{x}})>$ is a constant over the spatial domain (Ω) and it will be the same as the ensemble average. Although random fields may be possibly cross-correlated, they are assumed to be statistically uncorrelated in this paper.

Among various analytical covariance functional forms, we adopted an exponential form as follows.

$$C(\vec{\boldsymbol{x}}_a, \vec{\boldsymbol{x}}_b) = \sigma^2 exp(-\frac{|x_a - x_b|}{L_x} - \frac{|y_a - y_b|}{L_y} - \frac{|z_a - z_b|}{L_z})\ \vec{\boldsymbol{x}}_a, \vec{\boldsymbol{x}}_b \in \Omega \tag{2}$$

where $\vec{\boldsymbol{x}}_a(x_a, y_a, z_a)$ and $\vec{\boldsymbol{x}}_b(x_b, y_b, z_b)$ are the position vectors for randomly selected two locations in the coordinate system; L_i is the correlation length in i-th direction; and σ is the standard deviation. Defining the different correlation lengths $L_x \neq L_y \neq L_z$ allows for direction-sensitive spatial correlation in Cartesian or any rotated coordinate system. The eigenvalue and eigenfunction (λ_i, ϕ_i) in Eq. (1) are determined by solving the following Fredholm integral equation

$$\int_{\Omega_{be}}^{1} C(\vec{\boldsymbol{x}}_a, \vec{\boldsymbol{x}}_b)\phi_i(\vec{\boldsymbol{x}}_b)dV_{be} = \lambda_i\phi_i(\vec{\boldsymbol{x}}_a) \tag{3}$$

where $dV_{be} = dx_b dy_b dz_b$ is the infinitesimal elemental volume; $\boldsymbol{\Omega}_{be}$ is the domain related to $\vec{\boldsymbol{x}}_b$. The Galerkin finite element method was used for discretizing Eq. (3) [48]. We used Lagrangian interpolation functions (N_j) for approximating the eigenfunction as follows.

$$\phi_i(\vec{\boldsymbol{x}}_b) = \sum_{j=1}^{nnod_{RF}} N_j(\vec{\boldsymbol{x}}_b)d_{ij} = \boldsymbol{N}(\vec{\boldsymbol{x}}_b)\mathbf{d_e} \tag{4}$$

where d_{ij} is the jth nodal value of the ith eigenfunction; $nnod_{RF}$ is the number of nodes per random field element, which is 20 in this paper. Substituting Eq. (4) to Eq. (3) and expressing the integral residual of Eq. (3) weighted by the interpolation function $\boldsymbol{N}(\vec{\boldsymbol{x}}_a)$,

$$\begin{aligned}&[\int_{\Omega_{ae}}\int_{\Omega_{be}} C(\vec{\boldsymbol{x}}_a, \vec{\boldsymbol{x}}_b)\boldsymbol{N}(\vec{\boldsymbol{x}}_a)^T\boldsymbol{N}(\vec{\boldsymbol{x}}_b)\,|\mathbf{J}_e|^2 dV_{be}dV_{ae}]\boldsymbol{d_e}\\ &= \lambda_i[\int_{\Omega_{ae}} \boldsymbol{N}(\vec{\boldsymbol{x}}_a)^T\boldsymbol{N}(\vec{\boldsymbol{x}}_a)|\mathbf{J}_e|dV_{ae}]\boldsymbol{d_e}\end{aligned} \tag{5}$$

where $|\mathbf{J}_e|$ is the determinant of the Jacobian matrix mapping from the isoparametric space to physical space. In an elemental matrix form, Eq. (5) can be written as

$$\mathrm{C_e d_e} = \lambda_i \mathrm{b_e d_e} \tag{6}$$

Assembling all random field elements, the generalized eigenvalue problem is expressed as follows.

$$\mathbf{CD} = \Lambda\mathbf{BD} \tag{7}$$

where

$$\boldsymbol{C} = \sum_{ae=1}^{\mathrm{NRF}}\sum_{be=1}^{\mathrm{NRF}}\int_{\Omega_{ae}}\int_{\Omega_{be}}^{1} C(\vec{\boldsymbol{x}}_a, \vec{\boldsymbol{x}}_b)\boldsymbol{N}(\vec{\boldsymbol{x}}_a)^T\boldsymbol{N}(\vec{\boldsymbol{x}}_b)\,|\mathbf{J}_e|^2 dV_{be}dV_{ae} \tag{8}$$

$$\Lambda_{\mathbf{ij}} = \delta_{ij}\lambda_i \tag{9}$$

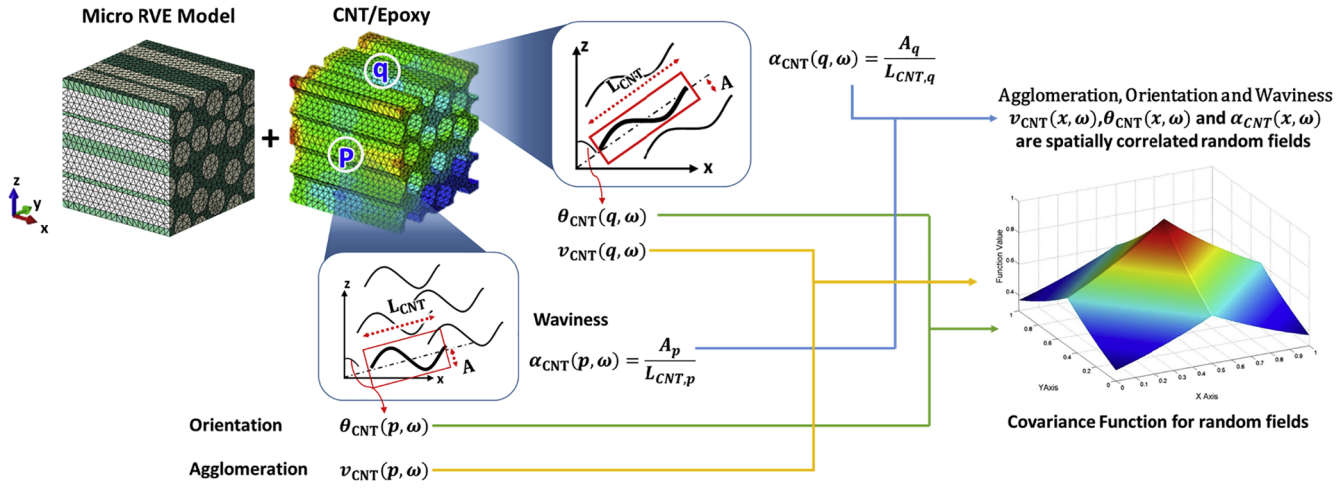

Fig. 1. Modeling of carbon fiber reinforced CNT/epoxy composite with spatial random properties.

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