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Three-dimensional microscopic assessment of randomly distributed representative volume elements for high fiber volume fraction unidirectional composites

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ABSTRACT

Generating realistic non-uniformly distributed three-dimensional representative volume element (RVE) for modeling the response of high fiber volume fraction composites is challenging. A novel rapid approach employing a random event-driven molecular dynamics simulation (EDMD) was proposed in this study for this purpose. Distributions of continuous unidirectional fibers in the RVEs were assessed using two approaches, namely Voronoi tessellations and radial distribution functions. The developed method was highly efficient in generating RVEs with realistic fiber dispersions. Furthermore, applying the corresponding periodic boundary conditions (PBCs) for finite element modeling is also arduous. A technique was developed within the commercial finite element software ABAQUS to rapidly produce required matching mesh patterns on opposite surfaces of the RVE, and to apply the corresponding PBCs using custom scripts. By coupling the EDMD approach and custom scripts within ABAQUS to rapidly generate and mesh RVEs with high fiber volume fractions, evaluation of the RVE response was greatly simplified. In- and out-of-plane elastic properties of unidirectional glass/epoxy composite in a range of 10–80% fiber volume fractions were determined and compared with analytical models, and available experimental data, with good correlation.

1. Introduction

Fiber-reinforced polymer (FRP) composite materials have been employed in many engineering applications, including aircraft and submarines, due to their merits in mechanical performance, such as high strength-to-weight and stiffness-to-weight ratios, excellent fatigue properties, and the ability to tailor their properties for specific applications. There are several variables that can be modified to tailor the properties of FRP composite materials, such as the lamina thickness, fiber volume fraction, fiber orientations, and fiber distribution [1–5]. As a result, efficient design tools are required to accurately assess the mechanical properties of various candidate material systems during the early stages of design, and for investigating local damage progression and predicting fracture of FRP composites.

There are three main methods used to determine the mechanical properties of composites, which include experimental measurements, micromechanical computational models, and analytical solutions. Experimental methods are costly and deemed generally impractical for preliminary design purposes, although they are required for evaluation of final material properties. Analytical models are generally suitable for assessing the elastic properties of FRPs, however, limitations exist when considering out-of-plane elastic properties such as shear modulus [6,7] or for assessing local damage evolution. In addition, some analytical models are complex and difficult to implement, while they are also limited in their ability to accurately capture the true microstructure of composites and nonlinear material behavior. Micromechanical computational models based on finite element method (FEM) provide an efficient means to conduct virtual experiments for various materials systems during design, while at the same time allowing for greater flexibility with regards to assessing material nonlinearities and local damage progression of FRPs. In this approach, a representative volume element (RVE) is utilized to represent the material microstructure, where practical complicated microstructures of composite materials can be simulated.

In a number of reported studies, the sophisticated microstructure of FRPs have been simplified using a single-fiber RVE and assuming a particular periodic distribution of fibers [8–13]. However, in order to accurately calculate mechanical properties and local stress

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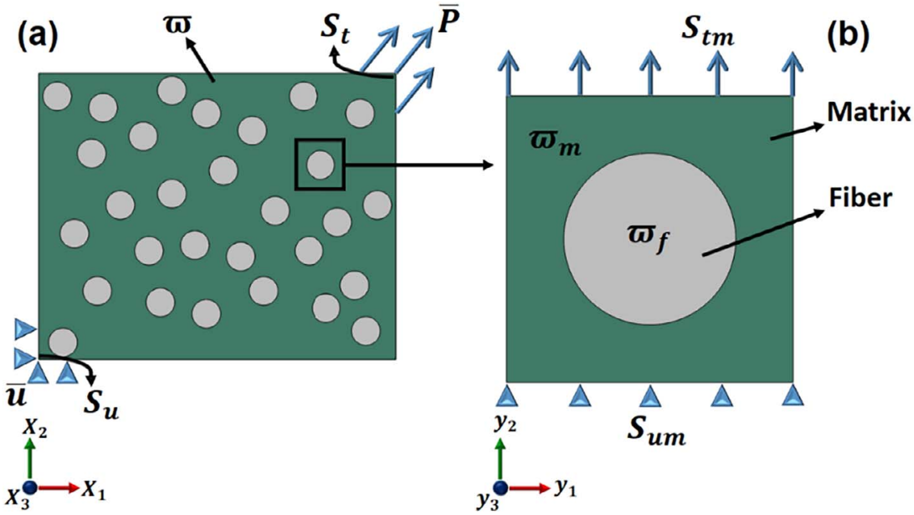

Fig. 1. (a) Non-homogenous periodic region of a UD glass/epoxy composite with volume ϖ under external boundary forces $\bar{P}$ and displacement $\bar{u}$; (b) a corresponding unit cell with fiber and matrix volume ϖ_f and ϖ_m respectively, S_{tm} and S_{um} are the exterior unit cell surfaces on which tractions and displacements are prescribed.

concentrations, and predict the onset and evolution of local damage, a practical non-uniform distribution of fibers must be considered [14,15]. One of the significant obstacles in modeling 3D multi-fiber RVEs is to randomly generate non-uniform fiber distributions efficiently, in particular for FRPs with high fiber volume fractions. In this regard, a number of algorithms have been developed [16–24]. The hard-core random distribution algorithm (HCRDA) was established by Yang et al. [16], while extensions such as the close packing model [17], stirring method [18,19] and random sequential expansion (RSE) algorithms [20] were also developed to overcome the jamming limitation of the HCRDA. The HCRDA is not efficient in generating RVEs with high fiber volume fractions [21]. The nearest neighbor algorithm (NNA) was later developed by Vaughan and McCarthy [22]. Due to the inter-fiber problem of NNA, the modified NNA (MNNA) was proposed by Wang et al. [23]. Furthermore, Zhang and Yan [24] proposed elastic collision algorithm (ECA). The principal drawback for the aforementioned algorithms is an inefficiency or inability to randomly generate RVEs with non-uniform dispersions and high fiber volume fractions.

A vigorous method for generating a high volume fraction of particles for any condition is through molecular dynamics simulations (MDS) [25]. A 2D packing of rigid disks with high volume fraction was generated using this method [26,27], however, the computational time required with conventional time-driven MDS is impractical [29]. In order to address this limitation, event-driven molecular dynamics (EDMD) or collision-driven molecular dynamics (CDMD) [28] have been proposed. However, EDMD algorithms have not been widely employed to generate RVEs for FRP composites.

With regards to micromechanical finite element (FE) modeling of FRPs, a large number of studies developed 2D RVEs with non-uniform fiber distributions and periodic boundary conditions (PBCs) [30–32]. However, a limitation with 2D RVEs includes an inability to assess out-of-plane mechanical properties of composites or 3D damage evolution under practical multiaxial stress states. Several studies have proposed 3D RVEs to investigate unidirectional (UD) composites. Qing and Mishnaevsky [33] generated a 3D RVE for UD composites with a simplified structured periodic fiber distribution. Recently, Ahmadian et al. [34] developed 3D RVEs with non-uniform distribution of fibers and periodic geometry for various fiber volume fractions up to 50%. However, they used complicated algorithms to generate the RVE geometry and develop the meshing scheme to ensure PBCs were applied to the FE model. A number of additional noteworthy contributions have been made by various groups using 3D RVEs for UD composites [35–41]. However, in most cases, the RVE geometry, fiber distribution or boundary conditions have been simplified, or the fiber volume fraction is less than 50%, which limits their applicability. In effect, in most practical applications, the volume fraction of UD composites is more than 50% [42–44,19,45]; for fabric-reinforced composites local tow fiber volume fractions may reach 80%. Therefore, to accurately assess the local damage evolution or 3D mechanical properties, an RVE with non-uniform fiber distribution and volume fraction greater than 50% is required. One of the difficulties lies in generating these RVEs and assessing as a periodic FE model.

Although the reported studies have made significant contributions in this field, assessment of UD fiber-reinforced composites with high fiber volume fractions using 3D RVEs with realistic non-uniform fiber distributions has not been widely explored and continues to be a challenge. Therefore, in this paper a novel and efficient method based on EDMD theory is proposed to randomly generate 3D RVEs for high fiber volume fraction UD composites with realistic microstructures (i.e., containing non-uniformly distributed fibers), which is the main contribution of this study. The goal is to develop a high-fidelity design tool for assessing the performance of high volume fraction UD composite materials. Moreover, an efficient algorithm is developed to create analogous mesh patterns on corresponding surfaces of the RVEs within the commercial FE software ABAQUS. A customized script was integrated to mesh and apply PBCs to the generated RVEs, thus simplifying the pre-processing stage of the analysis and ensuring rapid generation of the FE models for high volume fraction UD composites. In order to determine the accuracy of the generated RVE microstructures, the elastic properties of UD glass/epoxy composites such as Young's modulus along three material directions (i.e., longitudinal (E_1) and transverse (E_2 and E_3)), in- and out-of-plane shear modulus (i.e., G_{12}, G_{13}, and G_{23}), and Poisson's ratios (i.e., ν_{12}, ν_{21}, ν_{13} and ν_{23}) for various volume fractions are predicted and compared to experimental data from the literature as well as predictions from established analytical models.

2. The theory of homogenization

In order to characterize mechanical properties of heterogeneous materials such as UD composites, a homogenization process depicted in Fig. 1 can be utilized [32,46]. For the generated micromechanical RVEs in this study, homogenization was an essential step for extracting the required bulk UD composite mechanical properties. In general, for a heterogeneous material, the equilibrium equations, strain–displacement relations, and constitutive law are defined as follows:

$$\sigma_{ij,j} + f_i = 0 \text{ in } \varpi, \quad (1)$$