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Multiscale modeling of regularly staggered carbon fibers embedded in nano-reinforced composites

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ABSTRACT

This article deals with the multiscale modeling of stress transfer characteristics of nano-reinforced polymer composite reinforced with regularly staggered carbon fibers. The distinctive feature of construction of nano-reinforced composite is such that the microscale carbon fibers are packed in hexagonal array in the carbon nanotube reinforced polymer matrix (CNRP). We considered three different cases of CNRP, in which carbon nanotubes (CNTs) are: (i) aligned along the direction of carbon fiber, (ii) aligned radially to the axis of carbon fiber, and (iii) randomly dispersed. Accordingly, multiscale models were developed. First, molecular dynamics (MD) simulations and then Mori-Tanaka technique were used to estimate the effective elastic properties of CNRP. Second, a micromechanical three-phase shear lag model was developed considering the staggering effect of microscale fibers and the application of radial loads on the cylindrical representative volume element (RVE) of nano-reinforced composite. Our results reveal that the stress transfer characteristics of the nano-reinforced composite are significantly improved by controlling the CNT morphology, particularly, when they are randomly dispersed around the microscale fiber. The results from the developed shear lag model were also validated with the finite element shear lag simulations and found to be in good agreement.

1. Introduction

Fiber-matrix interfacial properties significantly affect the structural performance of composites subjected to external loads. The ability to tailor fiber-matrix interfacial properties is essential to ensure efficient load transfer from matrix to the fibers, which help to reduce stress concentrations and damage, and enhance overall mechanical behavior of resulting composite (Zhang et al., 2012). Several experimental and analytical techniques have been developed thus far to gain insights into the basic mechanisms dominating the fiber-matrix interfacial characteristics because the strength and toughness of the composite is largely dependent on the nature of fiber-matrix interface. To characterize stress transfer mechanisms, the pull-out test or shear lag model is typically employed. A significant number of analytical and computational two- and three-phase shear lag models have been developed to better understand the stress transfer mechanisms across the fiber-matrix interface (Gao and Li, 2005; He et al., 1999; Kundalwal et al., 2014; Li and Saigal, 2007; Nairn, 1997). These models differ in terms of whether the interphase between the fiber and the matrix is considered or not, and whether we are concerned with long fiber or short fiber composites. In the case of three-phase shear lag model, a thin interphase formed as a result of chemical interactions between the fiber and the matrix, is considered. The chemical composition of such interphase differs from both the fiber and matrix constituents but its mechanical properties lie between these two (Drzal, 1986; Kundalwal and Meguid, 2015; Sottos et al., 1992), and such nanoscale interphase has a marginal influence on the bulk elastic properties of a composite. On the other hand, a third phase (that is, relatively thick interphase) made of different material can be engineered between the fiber and the matrix (Kundalwal et al., 2014; Ray and Kundalwal, 2014). Such microscale interphase strongly influences the mechanical and interfacial properties of a composite, where the reinforcing effect is related to the interfacial adhesion strength, and the interphase serving to inhibit crack propagation or as mechanical damping elements [see (Zhang et al., 2010a) and the references therein].

CNTs (Iijima, 1991) have been emerged as the ideal candidates for multifarious applications due to their remarkable elastic and physical properties. A CNT can be viewed as a hollow seamless

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cylinder formed by rolling a graphene sheet. A significant number of experimental and numerical studies have been carried out to estimate the elastic properties of CNTs (Gupta et al., 2010; Kundalwal and Kumar, 2016; Krishnan et al., 1998; Shen and Li, 2004; Treacy et al., 1996), and reported that the axial Young's modulus of CNTs is in the TeraPascal range. The quest for utilizing such exceptional elastic properties of CNTs has led to the opening of an emerging area of research concerned with the development of two-phase CNT-reinforced nanocomposites (Chatzigeorgiou et al., 2012; Kundalwal and Meguid, 2015; Liu and Chen, 2003; Wernik and Meguid, 2010). However, the addition of CNTs in polymer matrix does not always result in improved effective properties of the two-phase nanocomposites. Several important factors, such as agglomeration, aggregation and waviness of CNTs, and difficulty in manufacturing also play a significant role (Wernik and Meguid, 2010). These difficulties can be alleviated by using CNTs as secondary reinforcements in a three-phase CNT-reinforced composite. Extensive research has been dedicated to the introduction of CNTs as the modifiers to the conventional composites in order to enhance their multifunctional properties. For example, Bekyarova et al. (2007) reported an approach to the development of advanced structural composites based on engineered CNT-microscale fiber reinforcement; the CNT-carbon fabric-epoxy composites showed ~30% enhancement of the interlaminar shear strength as compared to that of microscale fiber-epoxy composites. Garcia et al. (2008) grew aligned CNTs (A-CNTs) on the circumferential surfaces of microfibers to reinforce the matrix and reported the improvement in multifunctional properties. Hung et al. (2009) fabricated unidirectional composite in which CNTs were directly grown on the circumferential surfaces of conventional microscale fibers. Davis et al. (2010) fabricated the carbon fiber reinforced composite incorporating functionalized CNTs in the epoxy matrix; as a consequence, they observed significant improvements in tensile strength, stiffness and resistance to failure due to cyclic loadings. Zhang et al. (2010a) deposited CNTs on the circumferential surfaces of electrically insulated glass fiber surfaces. According to their fragmentation test results, the incorporation of an interphase with a small number of CNTs around the fiber, remarkably improved the interfacial shear strength of the fiber-epoxy composite. The functionalized CNTs were incorporated by Davis et al. (2011) at the fiber/fabric–matrix interfaces of a carbon fiber-epoxy composite; their study showed improvements in the tensile strength and stiffness, and resistance to tension–tension fatigue damage due to the created CNT- reinforced region at the fiber/fabric–matrix interfaces. Pavia and Curtin (2012) developed a shear lag model for a ceramic matrix composite containing wavy, finite length nanofibers having a statistical distribution of strengths as a function of all the material parameters including morphology. A numerical method is proposed by Jia et al. (2014) to theoretically investigate the pull-out of a hybrid fiber coated with CNTs. They developed two-step finite element (FE) approach: a single CNT pull-out from the matrix at microscale and the pull-out of the hybrid fiber at macroscale. Their numerical results indicate that the apparent interfacial shear strength of the hybrid fiber and the specific pull-out energy are significantly increased due to the additional bonding of the CNT–matrix interface. A beneficial interfacial effect of the presence of CNTs on the circumferential surface of the microscale fiber samples is demonstrated by Jin et al. (2014) resulting in an increase in the interlaminar shear strength (>30 MPa) over uncoated samples. This increase is attributed to an enhanced contact between the resin and the fibers due to an increased surface area as a result of the CNTs. Recently, current authors (Kundalwal et al., 2014) investigated the stress transfer characteristics of a novel hybrid hierarchical nanocomposite in which the carbon fibers augmented with CNTs on their circumferential surfaces are interlaced in the polymer matrix. They developed micromechanics models to determine the elastic properties of CNRP phase and the stress transfer characteristics of hybrid composite. Two types of CNT morphologies are studied by Romanov et al. (2015): CNTs deposited in fiber coatings and CNTs grown on circumferential surfaces of fibers. In the former case CNTs are tangentially aligned along the fiber surface and are radially aligned in the latter case. Most recently, the improved mechanical properties and stress transfer behavior of multiscale composite containing nano- and micro-scale reinforcements is reported by Kundalwal and Kumar (2016). They developed three-phase pull-out model to analyze the stress transfer characteristics within a single cylindrical RVE, neglecting the staggering effect of adjacent RVEs.

Findings in the literature indicate that the use of CNTs and conventional microscale fibers together, as multiscale reinforcements, significantly improve the overall properties of resulting hybrid composites, which are unachievable in conventional composites. It is well known that damage initiation is progressive with the applied load and that the small crack at the fiber-matrix interface may reduce the fatigue life of composites. By toughening the interfacial fiber-matrix region with nano-fillers, we can enhance the long-term performance as well as damage initiation threshold of conventional composites. Indeed, this concept can be exploited to grade the bulk matrix properties around the conventional fibers, which may eventually improve the stress transfer behavior of multiscale composite. To the best of our knowledge, there has been no multiscale model to study the stress transfer characteristics of nano-reinforced composite containing orthotropic micro- and nano-scale fillers. Existing shear lag models are insufficient to accurately describe the stress transfer mechanisms because they model the interactions among constituents at different scales through analytical or numerical micromechanical techniques. This provides the motivation behind the current study. Therefore, a more comprehensive multiscale model was advanced in this study to investigate the stress transfer mechanisms of nano-reinforced composite, in which the effects of different scales of constituents were taken into account. First, we developed multiscale model to determine the orthotropic elastic properties of CNRP through MD simulations in conjunction with the Mori-Tanaka model. The resulting intermediate CNRP phase, containing CNTs and epoxy, was considered as an interphase. Then the determined elastic moduli of the CNRP were used in the development of three-phase shear lag model accounting staggering effect of adjacent RVEs. Particular attention was paid to investigate (i) the influence of orientation of CNTs, and (ii) the effect of variation of the axial and lateral spacing between the adjacent microscale fibers on the stress transfer characteristics of the composite.

2. Multiscale modeling

For most multiscale composites, mechanical response and fracture behavior arise from the properties of its different constituents at each level and the interaction between these constituents. Thus, different multiscale models have been developed over the last decade to predict the overall properties of composites at the microscale level [Alian et al. (2015a, b) and the references therein]. Here, multiscale modeling of a nano-reinforced composite was achieved in two consecutive steps: (i) orthotropic elastic properties of the nano-fiber made of a single CNT and the epoxy matrix were determined through MD simulations; (ii) the determined elastic properties of the nano-fiber and epoxy were used to determine the bulk elastic properties of the CNRP using Mori-Tanaka model. Fig. 1 shows the steps involved in the hierarchical multiscale model.