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Multiscale modeling of stress transfer in continuous microscale fiber reinforced composites with nano-engineered interphase

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ABSTRACT

This study is focused on the mechanical properties and stress transfer behavior of multiscale composites containing nano- and micro-scale reinforcements. The distinctive feature of construction of this composite is such that the carbon nanostructures (CNS) are dispersed in the matrix around the continuous microscale fiber to modify microfiber-matrix interfacial adhesion. Such CNS are considered to be made of aligned CNTs (A-CNTs). Accordingly, multiscale models are developed for such hybrid composites. First, molecular dynamics simulations in conjunction with the Mori-Tanaka method are used to determine the effective elastic properties of nano-engineered interphase layer composed of CNS and epoxy. Subsequently, a micromechanical pull-out model for a continuous fiber multi-scale composite is developed, and stress transfer behavior is studied for different orientations of CNS considering their perfect and imperfect interfacial bonding conditions with the surrounding epoxy. Such interface condition was modeled using the linear spring layer model with a continuous traction but a displacement jump. The current pull-out model accounts for the radial as well as the axial deformations of different orthotropic constituent phases of the multiscale composite. The results from the developed pull-out model are compared with those of the finite element analyses and are found to be in good agreement. Our results reveal that the stress transfer characteristics of the multiscale composite are significantly improved by controlling the CNT morphology around the fiber, particularly, when they are aligned along the axial direction of the microscale fiber. The results also show that the CNS-epoxy interface weakening significantly influences the radial stress along the length of the microscale fiber.

1. Introduction

The structural performance of a composite under service load is largely affected by the fiber-matrix interfacial properties. The ability to tailor interfacial properties is essential to ensure efficient load transfer from matrix to the reinforcing fibers, which help to reduce stress concentrations and improve overall mechanical properties of a 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. The strength and toughness of the resulting composite is dependent on two facts: (i) efficient stress transfer from matrix to fiber, and (ii) the nature of fiber-matrix interface. To characterize these issues, the pull-out test or shear lag model is typically employed. A number of analytical and computational two- and three-cylinder pull-out models have been developed to better understand the stress transfer mechanisms across the fiber-matrix interface (Kim et al., 1992, 1994; Tsai and Kim, 1996; Quek and Yue, 1997; Fu et al., 2000; Fu and Lauke, 2000; Banholzer et al., 2005; Ahmed and Keng, 2012; Meng and Wang, 2015; Upadhyaya and Kumar, 2015). 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 or short fiber composites. In the case of three-cylinder pull-out model, a thin layer of interphase, formed as a result of physical and chemical interactions between the fiber and the matrix, is considered. The chemical composition of such an interphase differs from both the fiber and matrix materials but its mechanical properties lie between those of the fiber and the matrix (Drzal, 1986; Sottos et al., 1992; Kundalwal and Meguid, 2015), and such nanoscale interphase has a marginal influence on the bulk elastic properties of a composite. On the other hand, a relatively thick interphase can be engineered between the fiber and the matrix, especially a third phase made of different material than the main constituent phases (see for e.g. Liljenhjerte and Kumar, 2015). Such microscale inter-

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phase strongly influences the mechanical and interfacial properties of a composite, where the apparent reinforcing effect is related to the cooperation of the interfacial adhesion strength, and the interphase serving to inhibit crack propagation or as mechanical damping elements [see Zhang et al. (2010) and the references therein].

Recently, CNTs and graphene have attracted intense research interest because of their remarkable electro-thermo-mechanical properties, which make them candidates as nano-fillers in composite materials (Chatzigeorgiou et al., 2012; Kundalwal et al., 2014; Pal and Kumar, 2016a,b; Cui et al., 2016; Arif et al., 2016; Kumar et al., 2016). Extensive research has been dedicated to the introduction of graphene and 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. Cho et al. (2007) modified the epoxy matrix in microscale fiber-epoxy composites with graphite nanoplatelets and reported the improved in-plane shear properties and compressive strength for the resulting hybrid composite. Garcia et al. (2008), Lachman et al. (2012) and Wicks et al. (2014) grew aligned CNTs (A-CNTs) on the circumferential surfaces of microfibers to reinforce the matrix and reported the improvement in composite delamination resistance, toughness, Mode I fracture toughness, interlaminar shear strength, matrix-dominated elastic properties and electrical conductivity. 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. (2010) 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 reinforced epoxy composite laminate material; 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. 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 maximum interlaminar shear strength (>30 MPa) compared to 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. To improve the interfacial properties of microscale fiber-epoxy composites, Chen et al. (2015) introduced a gradient interphase reinforced by graphene sheets between microscale fibers and matrix using a liquid phase deposition strategy; due to the formation of this gradient interphase, 28.3% enhancement in interlaminar shear strength of unidirectional microscale fiber-epoxy composites is observed with 1wt%, loading of graphene sheets. Recently, two types of morphologies are investigated by Romanov et al. (2015): CNTs grown on fibers and CNTs deposited in fiber coatings. The difference in the two cases is the orientation of CNTs near the fiber interface: radial for grown CNTs and tangent for CNTs in the coatings.

Findings in the literature indicate that the use of nano-fillers and conventional microscale fibers together, as multiscale reinforcements, significantly improve the overall properties of multiscale composites, which are unachievable in conventional composites. As is well known, 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 increase the damage initiation threshold and long-term reliability of conventional composites. This concept can be utilized to grade the matrix properties around the microscale fiber, which may eventually improve the stress transfer behavior of multiscale composite. To the best of our knowledge, there has been no pull-out model to study the stress transfer characteristics of multiscale composite containing transversely isotropic nano- and micro-scale fillers. This is indeed the motivation behind the current study. The current study is devoted to the development of a pull-out model for analyzing the stress transfer characteristics of multiscale composite. A-CNT bundles reinforced in the polymer (epoxy thermoset) material is considered as a special case of carbon nanostructures (CNS) embedded between the fiber and matrix, most relevant to bundling of single-wall carbon nanotubes (SWCNTs); the resulting intermediate phase, containing CNS and epoxy, is considered as an interphase. First, we carried out multiscale study to determine the transversely isotropic elastic properties of an interphase through MD simulations in conjunction with the Mori-Tanaka model. Then the determined elastic moduli of the interphase are used in the development of three-phase pull-out model. Particular attention is paid to investigate the effect of orientations of CNS considering their perfect and imperfect interfacial bonding conditions with the surrounding epoxy on the stress transfer characteristics of multiscale composite.

2. Multiscale modeling

For most multiscale composites, mechanical response and fracture behavior arise from the properties of the individual constituents at each level as well as from the interaction between these constituents across different length scales. As a consequence, different multiscale modeling techniques have been developed over the last decade to predict the continuum properties of composites at the microscale (Tsai et al., 2010; Yang et al., 2012; Alian et al., 2015a,b). Here, multiscale modeling of CNS-reinforced epoxy interphase is achieved in two consecutive steps: (i) elastic properties of the CNS comprised of a bundle of CNTs and epoxy molecules are evaluated using molecular dynamics (MD) simulations; (ii) the Mori–Tanaka method is then used to calculate the bulk effective properties of the nano-engineered interphase layer.

2.1. Molecular modeling

This section describes the procedure for building a series of MD models for the epoxy and the CNS. The technique for creating an epoxy and CNS is described first, followed by the MD simulations for determining the isotropic elastic properties of the epoxy material and the transversely isotropic elastic properties of the CNS. All MD simulations runs are conducted with large-scale atomic/molecular massively parallel simulator (LAMMPS; Plimpton, 1995). The consistent valence force field (CVFF; Dauber-Osguthorpe et al., 1998) is used to describe the atomic interactions between different atoms. The CVFF has been used by several researchers to model the CNTs and their composite systems (Tunvir et al., 2008;