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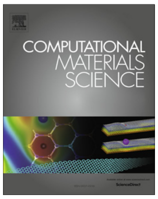

Multiscale modeling of the effect of waviness and agglomeration of CNTs on the elastic properties of nanocomposites

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ABSTRACT

In this paper, a multiscale model, based on molecular dynamics (MD) simulations and micromechanics modeling technique, was developed to determine the effect of waviness and agglomeration of CNTs on the bulk elastic properties of nanoreinforced epoxy composites. The predictions of most existing multiscale models overestimated the elastic properties of nanocomposites. We believe this difference is attributed to the unrealistic assumption that CNTs are straight reinforcements, which is contrary to the experimental findings. We overcame this limitation by using more realistic wavy CNTs. Representative volume elements (RVEs) reinforced with single and bundles of wavy CNTs were developed to study the effect of waviness, agglomeration, and orientation of CNTs on the bulk properties of the nanocomposite considered. CNTs with different curvatures ranging from straight to severely curved were modeled. Our results reveal that waviness and agglomeration of CNTs limit their reinforcement effects. The predictions of the proposed multiscale model are in very good agreement with existing experimental findings, verifying its validity and reliability.

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1. Introduction

Owing to their remarkable mechanical and physical properties, it is believed that few weight percentages of CNTs can significantly improve the mechanical, electrical, and thermal properties of CNT-based composites [1–3]. Such composites have found their way into different industrial applications such as electrostatic-assisted painting and electromagnetic interference shielding in automotive and aerospace industries, load-bearing applications in sporting goods industry, and in wind turbine blades and security boats [4]. More advanced applications that require multifunctional materials are being explored including structural health monitoring and lightning-strike protection for aerospace vehicles [4,5].

A significant number of experimental, numerical, and theoretical studies have been conducted to investigate the potential use of CNTs as reinforcing fibers [6,7]. Sun and Meguid [8] studied experimentally the tensile debonding of epoxy reinforced with homogeneously dispersed CNTs. Their results showed an improvement in the mechanical properties only at lower CNT concentrations, as at higher weight fractions the dispersed CNTs tend to agglomerate and aggregate. Allaoui et al. [9] significantly enhanced the mechanical properties of MWCNT–epoxy composites with 200% increase in Young's modulus over the pure epoxy with only 1 wt% of CNTs. Li et al. [10] managed to fabricate CNT–reinforced epoxy composites with relatively higher weight fractions of CNTs and found significant improvement in the mechanical properties. Their results showed that at 5 wt% of CNTs, Young's modulus increased from 4 to 7 GPa. The achieved improvement in the mechanical properties of CNT reinforced polymer composites is bounded by many factors such as uniform distribution, agglomeration, waviness of CNTs, and the strength of the interface between the embedded CNTs and the surrounding matrix. To study the influence of these parameters on the overall behavior of nanocomposites, several multiscale models have been developed; see e.g. Ref. [11]. In general, multiscale modeling of nanocomposites can be achieved in two consecutive steps. First, at the nanoscale level, MD simulation [12] or atomistic based continuum (ABC) techniques [13] can be used to obtain the atomic-level effective elastic properties of a representative volume element (RVE) consisting of a CNT embedded in a matrix. Second, at the bulk level, analytical and numerical micromechanical models are used to scale up the nanoscale properties to the microscale-level, leading to the bulk properties of the nanoreinforced composite [6,7,11].

Despite the remarkable elastic properties of CNTs, the reported experimental results in the literature show a limited enhancement

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in the effective elastic properties of their nanocomposites compared to the numerical and theoretical predictions [6,11,14]. The limited enhancement in the properties is attributed to different parameters: (i) agglomeration and aggregation of CNTs, (ii) poor interfacial properties, and (iii) CNT waviness, orientation, and quality (i.e. purities, and aspect ratios) [11–16]. The presence of agglomerates limits the reinforcement effect of the strong individual CNTs and leads to a nanocomposite with inferior properties [18]. This can be attributed to the rapid decrease in the strength of the CNT bundle due to the slippage of the CNTs within the bundle. This slippage limits the stress transfer between the CNTs within the bundle as well as between the CNTs and the surrounding polymer matrix [18]. The dispersed CNTs in the synthesized composite usually have some curvature due to their extremely high aspect ratio and very low bending stiffness [17]. Due to their high flexibility, CNTs tend to bend or unfold when dispersed in polymer matrices, as shown in Fig. 1 [11,14,19]. The processing of such nanocomposites usually includes a mixing step that uses both mechanical steering and sonication processes to homogenously disperse CNTs and break up their agglomerates in the prepared composites [1]. Due to the induced curvature, the elastic moduli of the CNTs and consequently the nanocomposite vary significantly in all directions [14]. For example, the reinforcing effect increases in the transverse direction and decreases in the chord direction with increasing CNT curvature [2].

Several experimental and theoretical studies have been conducted to investigate the effects of CNT agglomeration and waviness on the mechanical properties of their polypropylene composites [16–22]. The average size of the CNT agglomerates was measured using atomic force microscopy and found to be ~200 nm, while the diameter of the individual MWCNTs was ~25 nm [20]. The presence of such agglomerates limits the stress transfer between the CNTs and the polymer, and leads to composites with reduced elastic moduli [20]. Shi et al. [21] were among the first group to theoretically study the effect of CNT waviness and agglomeration on the elastic properties of CNT–polymer composites using micromechanics. The effective properties of nanocomposites reinforced with either helical CNT or spherical CNT agglomerates were obtained. Their results showed that both waviness and agglomeration degrade the bulk properties of the nanocomposite significantly. Weidt and Figiel [22] developed a 3D finite element (FE) model to predict the compressive behavior of epoxy matrix reinforced with curved CNTs. The properties of the CNTs and the CNT–polymer interface were determined using MD simulations. The waviness of CNTs was found to reduce the elastic modulus and the yield strength of the nanocomposite. On the other hand, micromechanical study by Dastgerdi et al. [16] revealed that wavy CNTs enhance the effective stiffness of the nanocomposite.

We believe that considering CNT waviness and agglomeration in multiscale modeling is very crucial for predicting the actual elastic properties of nanocomposite materials [11,14]. Previous models that considered polymer nanocomposites reinforced with isolated well-dispersed straight CNTs predicted mechanical properties that are much higher than the experimental measurements. To overcome this simplified model, many researchers developed micromechanical and FE models that consider wavy and agglomerated CNTs. However, most of these models considered perfect bonding between the matrix and the reinforcing CNTs and neglected the discrete nature of the constituents at the nanoscale level. CNTs were consistently assumed in these models as solid cylinders with isotropic or transversely isotropic properties [11,14] with limited consideration to the size effect.

From the above literature review, it can be concluded that a reliable model that considers these stated imperfections at the atomic level is highly desirable as it will overcome the inherited and artificially imposed limitations. To the best of the authors' knowledge, they are unware of any comparable studies. The present study is intended to fill this gap in the literature. It considers a multiscale model, based on MD simulations and micromechanical modeling techniques, to evaluate the effect of CNT waviness and agglomeration on the elastic properties of CNT–polymer nanocomposites. First, MD simulations of a wavy CNT embedded in an epoxy matrix were conducted to determine the effective elastic moduli at the nanoscale. Then, Mori–Tanaka micromechanical technique was used to scale up the nanoscale properties to the microscale level. The obtained numerical results were validated with recently obtained experimental findings.

2. Multiscale modeling

In order to design nanocomposites properly and optimize their properties, the effect of all parameters, including CNT waviness and agglomeration, on their performance must be considered. Controlling such parameters experimentally can be quite difficult and intricate. Therefore, a reliable multiscale model that accounts for all imperfections is highly desirable. In this study, a new multiscale model based on MD simulations and micromechanical modeling is developed in two steps to determine the effects of CNT waviness and agglomeration. The bulk properties of the nanocomposite are obtained in two consecutive steps. First, MD simulations were used to determine the stiffness tensors of the neat epoxy and the epoxy matrix reinforced with CNTs. CNTs with different curvatures were considered, while the agglomeration effect was captured by considering CNT bundles. Second, Mori-Tanka micromechanical technique was used to scale up the obtained nanoscale properties. Fig. 2 shows the steps involved in the hierarchical multiscale model.

2.1. Molecular dynamics simulations

In the present study, MD simulations were used to determine the effective elastic properties of the nanocomposite. All MD simulations were conducted with large-scale atomic/molecular massively parallel simulator (LAMMPS) [23] using the consistent valence force field (CVFF) [24]. This force field has been successfully used to predict the elastic properties of CNTs and epoxy polymers [12,25–28]. All interactions between the CNT and the polymer molecules were nonbonded interactions that originate from the van der Waals (vdW) interactions and electrostatic forces. The cut-off distance for these interactions was set to 14.0 Å [29]. Periodic boundary conditions were imposed on all directions of the RVE [30].

2.1.1. Modeling of epoxy matrix

Epoxy matrix based on DGEBA resin and TETA curing agent was used in the current study (see Fig. 3). From our past experience with the epoxy and to obtain the desirable elastic properties, the resin:curing agent weight ratio in the epoxy was set to 2:1. The details of the curing process and cross-linking procedures can be found in [12]. Each cured epoxy structure consists of 80 DGEBA molecules cross-linked with 40 molecules of curing agent TETA. This cross-linked epoxy structure was then used to build the epoxy system in the subsequent MD simulations. The properties of the neat epoxy are taken from our earlier MD study [12].

2.1.2. Modeling of nanocomposite reinforced with wavy CNTs

MD simulations were conducted for RVEs reinforced with wavy CNTs of different curvatures, as shown in Fig. 4. In the proposed model, CNTs were considered to have a sinusoidal shape as defined by:

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