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Mechanical properties and fracture analysis of functionalized carbon nanotube embedded by polymer matrix

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A B S T R A C T

There is no doubt about the importance of mechanical properties of polymer nanocomposite reinforced by carbon nanotubes (CNTs) in terms of the exclusive characteristic of both polymer and CNTs. The performance of carbon nanotubes polymer nanocomposite (CNTPN) depends on the interfacial characteristic between CNTs and polymer matrix. CNT functionalization process is a method for improving this characteristic. On the other hand, CNT functionalized method causes structural defects on CNT's structure. To have a more effective investigation on this process consequences of mechanical properties for the first time, several RVEs have been defined which incorporate effective parameters such as nonlinear structure of CNTs, nonlinear vdW interaction, nonlinear covalent bonds, fracture in polymer matrix, and structural defects into CNTs simultaneously. Also, RVEs are stiffed by long and short capped CNTs. In order to have a more realistic boundary condition, a new boundary condition is defined and it is found that not only functionalization process improves load transfer capability of RVEs, but also RVEs' ultimate strength is significantly increased as one of their functions, the covalent bonds are used to block debonding progress between CNT and polymer matrix. On the contrary, no improvement in Young's modulus is investigated during the functionalization process. Opposite to the RVEs including functionalized CNTs, an increase in polymer's ultimate stress causes the fracture mechanism in RVEs including intact CNTs to be completely changed. In addition, the interfacial shear stress (ISS) developed by pull-out CNT from the polymer matrix was studied to evaluate the effect of covalent bonds. The results revealed an improvement in the interfacial characteristic of RVEs. Moreover, the mean ISS was observed to be significantly improved. Mechanical properties of the equivalent nonlinear long RVEs for both armchair and zigzag stiffeners were demonstrated in tension, bending, and torsion conditions. The results also showed that linear beam elements presented accurate properties for equivalent beam only in a very small strain.

1. Introduction

Materials play a key role in every field of technology to make our lives more comfortable. This fact highlights the importance of development in materials science for having a better life in future. In order to create new generation materials, it is necessary to understand the relationship between the existing materials as well as their structure; thus, by combining appropriate materials, the desired properties are achievable [1].

The revolution in polymer nanocomposite has been brought by the discovery of CNTs in 1991 [2]. The first carbon nanotube reinforced nanocomposite was reported by Ajayan et al. [3]. Carbonaceous nanofillers, especially carbon nanotubes, play a very promising role due to their better structural and functional properties such as high stiffness, high strength, high aspect ratio, electrical conductivity etc. than others [4,5]. Polymers are the most suitable materials due to their low cost, reproducibility, easy processing, etc. Therefore, the combination of polymer matrix and CNT nanofillers is an opportunity for future materials in biomechanics, nanostructures, aerospace technology, etc. [6–8].

Both positive and negative effects of CNTs on polymer matrix have been reported in different studies [9]. Bhattacharyya et al. [10], Jia et al. [11], and Lau and Shi [12] have reported a decrease in mechanical properties when CNTs are added to the polymer. Some studies have represented an improvement in Young's modulus, but no improvement in the strength of polymer nanocomposite [13,14]. Using a nanoscale RVE based on the finite element method, Liu and Chen demonstrated that with additions of the CNTs in a matrix at volume fractions of only about 2% and 5%, the stiffness of the composite can increase up to 0.7 and 9.7 times for

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the short and long CNT cases, respectively [15]. On the contrary, several other studies have published the significant improvement of polymer's mechanical properties by adding CNTs as stiffeners [16–20].

One of the most effective parameters which significantly improves both Young's modulus and strength of carbon nanotube polymer nanocomposite (CNTPN) is the interaction between CNTs and polymer matrix [21–23]. Load caring capacity of CNTs and interfacial adhesion in CNTs/polymer nanocomposite has been extensively studied. It has been concluded that reinforcement significantly depends on the interfacial interaction between polymer and CNTs [22,24,25]. Therefore, several approaches such covalent functionalization have been used to enhance the properties of CNTPN [1,26], which is of more concern in this paper.

Functionalization is based on covalent linkages between carbon nanotube and other functional groups. Functionalization of CNTs may take place at the end caps and defect on the side walls [27, 28]. Although functionalization improves the interfacial interaction between CNTs and polymer, it creates several structural defects on CNT structures [29,30]. These defects decrease both Young's modulus and strength of CNTs significantly [24].

Several studies have been published to study the interfacial interaction between CNTs and polymer using RVE [31]. Li and Chou developed the multiscale modeling of the compressive behavior of CNTPN. The van der Waals (vdW) interaction between CNT atoms and the matrix was applied by truss elements [32]. A hybrid atomistic/continuum mechanics method for studying the deformation and fracture behavior of CNTs embedded in the matrix was presented by Shi et al. [33]. An equivalent continuum modeling method was developed to model nano-structured materials by Odegard et al. [34]. Tserpes et al. presented an RVE for modeling the tensile behavior of carbon nanotube–reinforced polymer nanocomposite. They considered intact CNTs with perfect bonds with polymer matrix. Wernik and Meguid presented the nonlinear response of armchair and zigzag nanotubes and their nanoreinforced polymer equivalents [35]. Shokrieh and Rafiee modeled the RVE with intact linear CNTs. The bonding between carbon nanotube and its surrounding polymer was considered nonlinear vdW interactions [36]. Ayatollahi et al. presented an equivalent beam element according to the nonlinear behavior of intact CNTs, then used the beam to build a cylindrical RVE [37]. Fereidoon et al. developed a multiscale FEM to study the interaction between CNTs and matrix near a crack. Mohammadpour et al. used contact elements to model the non-bonded interface [38]. Zuberi and Esat compared two non-bonded and perfectly bonded interaction between CNTs and polymer matrix [39]. Weidt and Figiel defined cohesive zone concept and adapted it to capture perfect and weak vdW bonding [40]. The effective material properties of the nanocomposite disk are estimated by a micro-mechanical model [41].

To have accurate RVE modeling, it is important to combine both improving effect of functionalization on interfacial interaction and decreasing effect of defects on the mechanical properties of CNTs. No computational model that incorporates the aforementioned aspects simultaneously and evaluates the effects of structural defect on the properties of polymer nanocomposite has yet been proposed. Hence, this work aims to develop a computational model that combines the effects of nonlinear behavior of CNTs in its lattice structure, structural defects, covalent bonds, and vdW force on the mechanical properties and fracture of CNTPN. Effects of covalent bonds on pull-out interfacial shear stress are also studied and the equivalent nonlinear properties of nonlinear beam elements are demonstrated for different CNTPNs.

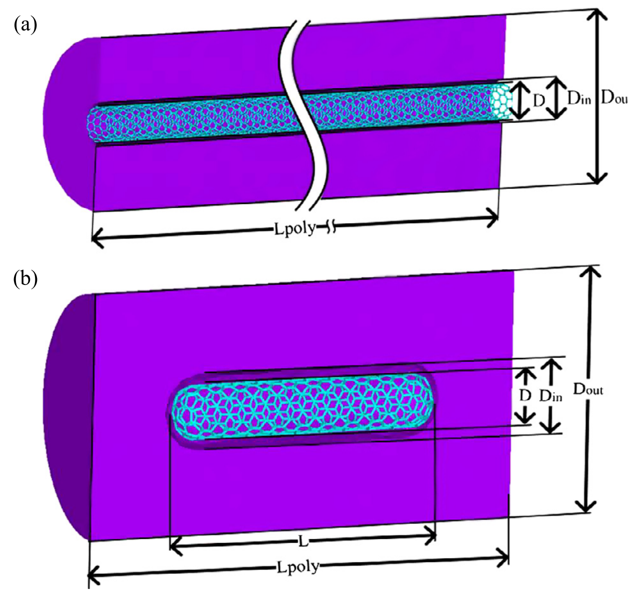

Fig. 1. RVEs with (a) long and (b) short CNTs.

2. Nonlinear finite element modeling of representative volume element (RVE)

Nonlinear cylindrical RVEs are developed using ANSYS commercial package. The primary aim of this RVE is to incorporate effective parameters in order to develop more accurate nanocomposite RVE modeling which has not been considered individually or in combination by previous works. These effective parameters are the nonlinear lattice structure of CNTs, nonlinear vdW interaction force, and nonlinear covalent bonds between defective functionalized CNTs and polymer matrix. In other words, the accuracy of RVE definitely depends on three parameters, accuracy of CNTs' computational model, modeling polymer phase, and realistic description about the interaction between these two phases. In this section, assumptions and computational models which affect these three parameters will be discussed.

Because of the geometrical similarity with CNTs, the cylindrical RVEs are more appropriate for the achievement of equivalent mechanical elements as suggested by other studies [36,38,39]. In Fig. 1, the nanocomposite RVEs are schematically shown. To study the effect of length on load transferring phenomena, two models of RVEs are constructed. In the first model, both polymer matrix and CNTs have the same length, whereas in the second one, the length of CNTs is smaller than that of the polymer.

Finite element models are constructed for CNTs, polymer, and interphase region as briefly discussed in this section.

2.1. CNT modeling

SWCNT is demonstrated as rolled graphene sheet. The diameter of an ideal carbon nanotube in Pico meter can be calculated as follows [42]:

$$d = \frac{a}{\pi}\sqrt{n^2 + nm + m^2} = 78.3\sqrt{(n+m)^2 - nm} \qquad (1)$$

where m and n are CNTs' chiral index and $a = 0.246$ [42].

In this study, the modified Morse is used as potential function. The energy potential function for Morse potential function is given as follows [24]:

$$E_{total} = U_r + U_\theta + U_\emptyset \qquad (2)$$

where respectively demonstrate energies associated with bond stretching, angle variation, torsion, and inversion as follows: