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Modeling the tensile stress–strain response of carbon nanotube/polypropylene nanocomposites using nonlinear representative volume element

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ABSTRACT

This paper presents a finite element model for predicting the mechanical behavior of polypropylene (PP) composites reinforced with carbon nanotubes (CNTs) at large deformation scale. Existing numerical models cannot predict composite behavior at large strains due to using simplified material properties and inefficient interfaces between CNT and polymer. In this work, nonlinear representative volume elements (RVE) of composite are prepared. These RVEs consist of CNT, PP matrix and non-bonded interface. The nonlinear material properties for CNT and polymer are adopted to solid elements. For the first time, the interface between CNT and matrix is simulated using contact elements. This interfacial model is capable enough to simulate wide range of interactions between CNT and polymer in large strains. The influence of adding CNT with different aspect ratio into PP is studied. The mechanical behavior of composites with different interfacial shear strength (ISS) is discussed. The success of this new model was verified by comparing the simulation results for RVEs with conducted experimental results. The results shows that the length of CNT and ISS values significantly affect the reinforcement phenomenon.

1. Introduction

Carbon nanotubes (CNTs) have attracted huge interest in most areas of engineering due to their unique physical and chemical properties. Carbon nanotubes are considered to be excellent reinforcement to improve toughness and fracture resistant [1], wear sliding [2], impact behavior [3] and thermal conductivity [4] of polymer composites. Experimental studies showed that the ability of carbon nanotubes to enhance the performance of polymer composites mostly depends on the strength of the interface and interactions between the polymer and CNTs [5,6]. The load carrying capacity of CNTs, polymer/CNT wetting and interfacial adhesion in CNT/polymer composites have been extensively studied using electron microscopy [7] and spectroscopic techniques [8]. Cadek et al. [6] studied the effects of interfacial surface area on the tensile behavior of poly(vinyl alcohol) films loaded with different types of CNTs. Results indicated that total nanotubes surface area is directly proportional to the tensile reinforcement. They concluded that reinforcement is significantly dependent on the interfacial interactions between polymer–CNTs. Advanced atomic force microscopy (AFM) method was used to understand and improve interfacial bonding between nanotubes and polymer [9]. They attempted to directly measure the interfacial energy between nanotubes and matrix. These observations demonstrated that the reinforcement potential of CNTs in composites can be substantial. Coleman et al. [10] discussed mechanical properties of CNTs, production and processing of composites in order to obtain system requirements for maximum mechanical performance.

While experimental studies in this field needs costly and time consuming characteristic tools, numerical approaches have been introduced to handle these investigations. Recent literature has shown that molecular dynamics and continuum simulations can play important roles in characterization of CNTs and CNT enabled composites [11]. Frankland et al. [12] studied the effect of functionalization on the nanotube/polymer shear strength using molecular dynamics (MD). Simulation of single-walled carbon nanotube (SWCNT) embedded in polyethylene matrix showed that shear strength at interface can be increased by chemical cross-linking between nanotube and polymer. Zheng et al. [13] simulated pullout of SWCNT from polymer matrix using molecular dynamics. They found out certain degree of functionalization may significantly increase the interfacial bonding between CNT and polymer.

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They characterized the interfacial shear strength of the composites and concluded that increasing load transfer between CNT and polymer may be an effective way to improve mechanical properties of the composites. The continuum mechanics has been also employed for more than a decay to characterize properties of CNTs [14]. In our recent numerical studies, see [15,16], on the mechanical behavior of CNTs we have demonstrated the potential application of finite element method. Furthermore, Liu and Chen have shown that finite element method is a feasible approach to obtain basic properties of CNT-based composites [17,18]. Unit cells of materials or representative volume elements (RVE) have been considered as a successful method in the studies of nanoscale properties of composites. Masud et al. [19] and Singh et al. [20] presented simplified nanoscale RVE models of CNT enabled composite in order to study the interphase properties and thermal conductivity of the composite, respectively. All these results suggested that interphase and volume fraction of CNTs has significant effect on nanocomposites behavior. Tserpes et al. [21] proposed a multiscale model for unidirectional nanotube/polymer composite based on continuum elasticity. They have developed separate models for CNT and polymer matrix. Their results showed that proper adhesion ensure the maximum load carrying capacity from polymer to the CNT. Prefect bonding at elastic range was also studied by Huang et al. [22] using truss and solid elements for CNT and polymer, respectively. They realized that CNT length has significant effect on the lateral deformation of the composite.

Research shows that interfacial region between the CNTs and polymer is an essential factor and challenging problem in all modeling approaches. Moreover, the correlations between the functional groups on the CNT wall, interfacial structure and load transfer mechanisms were studied in CNT/epoxy composites [23]. Their strain sensitive Raman spectroscopy studies of the samples under tension showed that several mechanism govern stress transfer behavior of the composites at different loading stages. Strong covalent bonding and weak mechanical/physical interactions between CNT and epoxy or a combination of them were suggested as the main load transfer mechanism in the composite. Tan et al. [24] incorporated a cohesive law established by Jiang et al. [25] to develop a nonlinear model for CNT/polymer interface derived from the van der Waals interactions. Their results revealed that mechanical behavior of composite at large strains is not sufficient due to completely debonded nanotubes which will behave like voids in the matrix.

Joint elements was employed to model imperfect bonding at CNT/polymer interface [26]. This parametric study confirmed the effect of a proper bonding between CNT and matrix. Shokrieh et al. [27] carried out a non-linear analysis on multi-scale RVE models consisted of CNT, polymer matrix and non-bonded interface. The nonlinear van der Waals interactions between CNT and polymer were simulated using spring elements. They showed that longer CNTs have stronger reinforcement capabilities in comparison with short CNTs. Another finite element model was proposed to estimate the effect of imperfect bonding on the tensile modulus of CNT-reinforced polypropylene (PP) composites [28]. They used atomic force microscope to characterize the CNT/PP contact area and defined an imperfect CNT/PP contact model.

Available literature shows that computational modeling tends to significantly over-predict the mechanical behavior of CNT/polymer composites, see for instance [17,27], mostly because they do not include experimental observations such as nonlinear material behavior at large strains. On the other hand, it is very difficult to account for the interfacial region between CNT and matrix in an efficient and accurate method. It seems neglecting materials and geometrical nonlinearity are important source of inaccuracy in current predictions [25]. Due to mentioned difficulties, the aim of present paper is to propose an effective model for CNT/polymer composites based on nonlinear finite element modeling. In this work, full 3-D nonlinear RVEs of CNT/polypropylene composite were developed to investigate the effects of CNT length and interfacial strength on the mechanical response of the composite. This RVE is an efficient tool in order to study the load transfer and interactions between CNTs and surrounding polymer. Stress and strain distributions in the components and the interface can be measured from the simulation results.

2. Experimental details

The polymer used in this study was Polypropylene (PP) provided by Titan Petchem (M) Sdn. Bhd. Multi-walled carbon nanotubes (MWCNTs) purchased from Shenzhen Nanotech Port Co., Ltd. The specifications of nanotubes as provided by the supplier were: outer diameter 40–60 nm, length 5–15 μm, purity >97% and ash less than 3%.

The nanocomposite samples were fabricated via melt mixing and injection molding. PP and the MWCNTs were mixed using the Haake Rheomix 600 mixer under temperatures of 200 °C, mixing speed of 30 rpm and a mixing duration of 15 min. And directly injection molded with the Krauss Maffei 40 Tonne injection molding machine into dog bone samples, adhering to the standard of ASTM: D638.

The stress–strain relationship and mechanical behavior of composite samples were determined with respect to CNT content according to ASTM: D638. For mechanical tests a 5 K universal testing machine were utilized with strain rate of 2 mm/min.

3. Finite element modeling

To evaluate the tensile properties of a CNT-based nanocomposite, cylindrical RVEs were developed using ANSYS software codes. The primarily goal is to present a more accurate and efficient model for nanocomposite. It is a common practice to assume all the composite phases uniform and isotropic in order to simulate their mechanical behavior [11]. It is assumed that the material is uniformly distributed in its volume at continuum level. The continuum material has an average density and can be subjected to surface forces [29,30]. Proper material models were integrated into elements to simulate structural and geometrical nonlinearities.

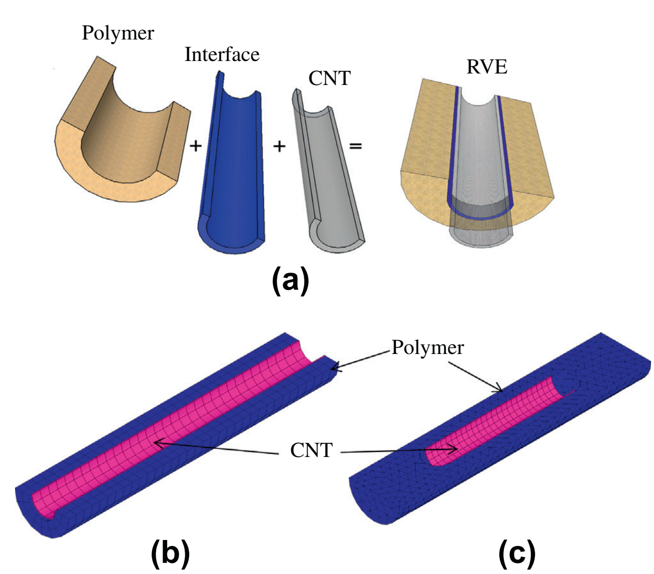

Fig. 1. (a) Schematic view of the present modeling technique, (b) RVE containing high aspect ratio CNT, (c) RVE containing low aspect ratio CNT.