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Molecular dynamics simulations of the single-walled carbon nanotubes/poly (phenylacetylene) nanocomposites

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ABSTRACT

The physical and mechanical properties of single-walled carbon nanotubes reinforced poly (phenylacetylene) are investigated here. Polymer density distribution, polymer atom distribution, stress–strain curve of single-walled carbon nanotubes/poly (phenylacetylene) and tensile and shear moduli of resulted nanocomposites are studied. It is shown that the polymer atom distribution at the nanotube/polymer interface is not uniform. It is observed that nanotube diameter and volume fraction do not affect polymer atom distribution around the single-walled carbon nanotubes significantly. Studying the effect of embedding nanotube in poly (phenylacetylene) on the tensile modulus of nanocomposite, it is shown that longitudinal Young's modulus is improved drastically. However, transverse moduli are not significantly improved compared to pure polymer.

1. Introduction

Recently, extraordinary mechanical, thermal, electrical and chemical properties of carbon nanotubes (CNTs) [1–3] have absorbed the interests of researchers to utilize them in polymer matrix nanocomposites. Specially, a great deal of works have been focused on improving the electrical

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conductivity [4–7], thermal conductivity [8,9] and mechanical properties [10–12] of polymer matrix by CNTs.

Some experimental approaches have been used to explore the mechanical properties of CNT/polymer nanocomposites [13–17]. However, due to the variety of factors which affect the mechanical properties of CNT reinforced nanocomposites, theoretical approaches are of great importance in exploring their mechanical behavior. The theoretical approaches, which have been used in this field, include atomistic simulations (such as molecular dynamics (MD) simulation), micromechanics approaches (such as role of mixtures, Mori–Tanaka, Tanaka and Halpin–Tsai) and finite element (FE) methods.

By using MD simulations, Frankland et al. [18] investigated the effect of embedding long and short single-walled carbon nanotube (SWCNT) in polyethylene on the mechanical properties of SWCNT/polyethylene nanocomposites. It was observed that long SWCNTs enhance the stiffness of nanocomposites as compared to pure polyethylene. However, no significant enhancement was observed for short SWCNTs. Han and Elliott [19] used MD simulations to study reinforcing poly(methyl methacrylate) (PMMA) and poly{(m -phenylene-vinylene)-co -[(2,5-dioctoxy- p-phenylene) vinylene]} (PmPV) with SWCNTs. Their results showed significant increase in the mechanical properties of polymer by embedding SWCNTs. The mechanical properties of SWCNT/Epon 862 nanocomposites were investigated by Zhu et al. [20]. They showed that reinforcing Epon 862 by long and short SWCNTs can improve the Young's modulus of the polymer about 1000% and 20%, respectively.

Mokashi et al. [21] modeled the SWCNT reinforced amorphous and crystalline polyethylene by means of MD simulations. It was shown that embedding SWCNTs in the crystalline polyethylene leads to moderate improvement on the mechanical properties relative to the pure polymer. However, for amorphous polyethylene, significant increase was observed. MD simulations were used by Tsai et al. [22] to assess the non-bonded gap and the non-bonded energy between the SWCNT and polyimide matrix. A three-phase micromechanical model was used to estimate the elastic properties of SWCNT/polyimide nanocomposites.

Based on MD simulations and continuum micromechanics, a multiscale method was proposed to study the elastic behavior of SWCNT/polypropylene nanocomposites by Yang et al. [23]. They also used a hierarchical multiscale model to explore the elastoplastic behavior of SWCNTs/polypropylene nanocomposites [24]. Besides, they employed MD simulations to study the effect of SWCNTs with Thrower–Stone–Wales (TSW) defects on the mechanical properties of nanocomposites. They reported that embedding defective SWCNTs in the polypropylene results in smaller longitudinal Young's modulus relative to using pristine SWCNTs. However, transverse Young's modulus and the transverse and longitudinal shear moduli are larger [25].

The mechanical properties of SWCNT/Poly (vinylidene fluoride) (PVDF) nanocomposites was investigated by Bohlén and Bolton [26]. Based on their results, the bulk and shear modulus properties of PVDF are not affected significantly by embedding SWCNTs. However, adding functionalized SWCNTs improves the mechanical properties of polymer more considerably.

FE methods are also being used vastly by different researchers to explore the mechanical properties of SWCNT/polymer nanocomposites. A FE-based multiscale method was used by Li and Chou [27] to study the compressive behavior of SWCNT reinforced nanocomposites. They used atomistic FE method to model the SWCNTs. The polymer was modeled by continuum FE method and truss element was employed to simulate the van der Waals (vdW) interactions between atoms of SWCNTs and polymers. A 3D FE was used by Shokrieh and Rafiee [28,29] to study the longitudinal, transverse and shear moduli of nanocomposites. Comparing the results of FE model with those of rule of mixture, they concluded that the latter approach cannot predict the mechanical properties of nanocomposites accurately. So, an equivalent fiber was developed by them to defeat this shortcoming.

The transition region from atomistic to continuum region was discussed by Wernik and Meguid [30]. Considering a nonlinear representative volume element (RVE) consisting of SWCNT, polymer matrix and SWCNT/polymer interface, they also used an atomistic-based continuum multiscale modeling technique to study the mechanical behavior of SWCNT/polymer nanocomposites [31]. A full atomistic FE model was used by Meguid et al. [32] to study the SWCNT reinforced epoxy RVEs. Using the developed homogenized RVE in a micromechanical analysis, they predicted the effective properties of SWCNT reinforced epoxies. The interfacial properties of SWCNT/polymer nanocomposites were explored by simulating the SWCNT pull-out [33].