



Self-densified microstructure and enhanced properties of carbon nanotube fiber by infiltrating polymer

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ARTICLE INFO

Article history:

Received 14 January 2016

Received in revised form

25 April 2016

Accepted 12 May 2016

Available online 13 May 2016

ABSTRACT

Polymer infiltration is an efficient way to strengthen carbon nanotube fibers in the process of spinning. Given the carbon nanotube/polymer composite fibers obtained from this approach possess higher mechanical properties than the ones of their components, the general rule of mixtures for a composite material is not applicable. Accordingly, a novel coarse-grained molecular dynamics model is proposed to investigate the mechanical behavior and microstructural evolution of the composite fibers, in which the carbon nanotubes and polymer chains are represented by mesoscale coarse-grained beads. Then the reinforcing mechanism of the composite fibers is illustrated. Dependence of the mechanical behavior on the microstructure of the composite fiber under different strain rates is revealed as well. Furthermore, the variations of mechanical properties of the composite fibers with cycle numbers under relatively low load are predicted.

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1. Introduction

Carbon nanotube (CNT) fibers have attracted enormous attention due to their hierarchical structure that transfers the superior properties of the individual CNTs at nanoscale to macroscale and realizes novel applications, such as torsional actuators [1–4] and sensors [5]. However, despite intensive efforts in advancing the spinning techniques, the mechanical properties of the neat CNT fibers still fall short of expectations [6–9]. It is established that the key factor hindering the strength improvement of the CNT fibers is the low shear interaction between the CNTs and their bundles, owing to inevitable pores, gaps, and defects between them [10].

In order to enhance the CNT fibers, long and well-aligned spinnable CNTs are highly desirable [11–14]. Besides, post-spin treatments can also be implemented to improve the CNT fibers, including twisting and shrinking [15], chemical functionalization [16], electron beam irradiation [17] or plasma [18], and infiltration of evaporable solvents or polymers [19]. Among these treatment methods, polymer infiltration provides a convenient and effective way for enhancing the as-spun CNT fibers without destroying the intrinsic structures of the CNTs.

To date, a variety of polymers with different molecular structures and sizes have been employed in the post-spin infiltration process for enhancing the CNT fibers [19–24]. According to the experimental results, CNT/polyvinyl alcohol (PVA) composite fibers exhibit significant reinforcement of mechanical properties than the neat CNT fibers [19–22]. Liu et al. [21] proposed an effective method of making high-strength CNT based composite fibers by using a super aligned CNT fiber as a framework and then inserting PVA into the intertube spaces of the framework to enhance the strength of yarns. The as-produced CNT/PVA composite yarns possess very high tensile strengths up to 2.0 GPa and Young's moduli more than 120 GPa. The enhancement of these composite fibers is mainly attributed to the cross-link network of the polymer chains that help enhancing the load transfer between the CNTs and their bundles and ameliorating their interfacial slippage. However, it has not been fully uncovered how the polymer chains interact with each other and with the CNTs in the composite fibers. Therefore, more detailed fundamental investigations are required for a better understanding of the enhancement of CNT/polymer composite fibers.

Coarse-grained (CG) models are powerful tools for studying the mechanical behavior of CNT-based materials [25–30]. In our previous work, coarse-grained molecular dynamics (CGMD) simulations have been performed to learn the mechanical behavior and microstructural evolution of the neat CNT fibers [25–27].

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Contribution factors such as length and alignment of the CNTs as well as the surface angle to the mechanical properties of the CNT fibers have been investigated. Lately, the improvement effect of post-spin twisting on the mechanical properties of the CNT fibers was revealed via CGMD simulations [30].

In this study, supplementary to experimental efforts to enhance CNT fibers, CGMD simulations can provide a powerful way to reveal the improved microstructure and microstructural evolution and fracture characteristics of the CNT/PVA composite fibers under tensile loading. The present CG models representing the single-walled CNTs and the PVA polymer chains are employed in the modeling of the CNT/PVA composite fibers, respectively. In particular, long chains of PVA polymer are chosen to study the effect of the cross-linked network on the mechanical properties of the CNT/PVA composite fibers. Forming of CNT/PVA composite fibers is reproduced by performing CGMD simulations of the polymer infiltration process. What's more, the stress-strain relations and microstructural evolution and fracture characteristics of the CNT/PVA composite fibers under monotonic and cyclic loadings are studied. The results are.

2. Method and models

The trajectories of all atoms are available from molecular dynamics (MD) simulations, providing information about every single molecule which are not easily detected from experiments. Nevertheless, performing full-atom MD simulations of a large system requires a huge amount of computation consumption. Accordingly, medium-scale CG models with structure and force potentials derived from the full-atom MD simulation results can provide both reasonable computational precision and efficiency simultaneously [31,32]. Moreover, in CGMD simulations, the microstructural evolution and mechanical properties of materials are obtained strictly based on the variation of total potential energy of the system, and are varied with different force field parameters and structures of the materials.

In this study, CG model for the CNT is the same as that was reported in our previous work [25–27], in which each CNT is represented by a string of beads connected by springs. Deformation of the CNTs are described by the change of the spring length and spring angle. Torsion of the CNTs has not been taken into account due to the fact that the CNTs are discontinuous in the fiber, and each CNT is free to rotate with respect to its axis. Hence, the total potential energy of the system is the sum of potential energies caused by stretching and bending of the springs, and the energies caused by van der Waals (vdW) interactions as well. However, different from the linear spring used in the previous CG model, a finite extensible nonlinear spring is introduced to better fit the actual force-strain response of the CNTs in this study. Therefore, the potential and force values of the spring as a function of spring length are interpolated from a table during the simulations. Besides, the elongation limit of the CNT spring is taken as 27 per cent in the present work [33]. Furthermore, CG model for the PVA polymer used in this work is also based on all-atom simulations, with force fields developed by using the program YASP reported by Reith et al. [34]. Models of amorphous PVA were obtained from Accelrys Material Studio. All the MD simulations were performed using the massively parallelized modeling code LAMMPS [35].

3. Results and discussion

3.1. Improved microstructure of CNT/PVA composite fiber

As observed by SEM in our previous work [36], the CNT fibers are mainly composed of numerous CNT bundles, which are formed

by self-assembly of the well-aligned CNTs. Hence, a model that can represent the unique morphology of the CNT fibers is built, as shown in Fig. 1. The fiber is formed by 7 hexagonally-arranged CNT bundles, each contains 19 hexagonally and densely packed CNTs with chirality of (5, 5). The diameter of each CNT is 0.68 nm, so the bundle size is 5.10 nm. A large amount of pores and spaces between the bundles are displayed on the surface of the fiber. The cross-sectional view of the CNT fiber is also given in Fig. 1b, showing slight bending of the inner CNT bundles. The length and the diameter of the CNT fiber are 600 nm and 34 nm, respectively. In total, there are 134,330 beads connected by 133,665 bonds in the present model. Therefore, the linear density of the CNT fiber is calculated as 0.33 tex (g/km), which is in the range of the experimental measurements of pristine CNT fibers [37–39]. In order to get an equilibrium morphology, the CNT fiber was placed in a box with periodic boundary conditions in three dimensions and relaxed at NPT ensemble (constant beads, constant pressure and constant temperature) with an applied isotropic pressure of 1 bar (1 bar = 10,000 Pa) for 500 ps at 298 K before performing simulations. What's more, a fixed timestep of 0.01 ps are used for all the simulations. It should be noted that the main purpose of this paper is to observe the change of CNT fiber structure during polymer infiltration and to analyze the dependence of microstructural evolution and fracture characteristics inside the CNT/PVA composite fiber on tensile strain rate. Therefore, due to the computational restrictions, the present simulations were performed on CNT fibers with given bundle size and fiber density, in which the CNTs are well-aligned.

Afterwards, CG model of the CNT/PVA composite fiber was obtained through infiltration of the CNT fiber by PVA polymer. As described in the previous experiments, the CNT fibers will be wrapped by a thin polymer layer on the surface after polymer infiltration treatment [40]. In order to reproduce this process, a cylinder tube filled up with PVA polymer was relaxed into the CNT fiber under a time-dependent radial pressure. The infiltration process was accomplished in 1 ns (100,000 steps), followed by fully relaxation of the system for 0.5 ns (50,000 steps). In this study, the polymer film is composed of 500 PVA chains, each contains 902 beads connected by 901 bonds. Therefore, the total numbers of the polymer beads and bonds are 451,000 and 450,000, respectively. Therefore, the linear density of the CNT/PVA composite fiber is calculated as 0.38 tex. As exhibited in Fig. 2, the diameter of the composite fiber is remarkably decreased from 40 nm to 30 nm after relaxation (the polymer chains are represented by blue lines while the CNTs are represented by black lines, and the dashed circle expresses the radial pressure applied on the composite fiber).

Therefore, microstructure of the closely packed CNT fiber after polymer infiltration was obtained. The CG model of the CNT/polymer composite fiber is given in Fig. 3a. The cross-sectional view of the composite fiber, as illustrated in Fig. 3b, demonstrates the infiltration of the polymer molecules into the outermost layers of the CNT fiber, which is consistent with the composite fiber as proposed by Liu et al. [40].

In order to explore the improvement of the microstructure of the CNT fiber after polymer infiltration, detailed images of the CNT



Fig. 1. Images of (a) CG model of neat CNT fiber and (b) its cross-sectional view.

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