



Superior interfacial mechanical properties of boron nitride-carbon nanotube reinforced nanocomposites: A molecular dynamics study



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HIGHLIGHTS

- Composites reinforced by BN-CNTs have superior interfacial shear strength (ISS).
- ISS of BN-CNT reinforced composites is larger than that of their CNT counterparts.
- ISS of BN-CNT reinforced composites depends on the BN composition of BN-CNTs.
- Superior ISS of the present composites is explained by classical friction theory.

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ABSTRACT

The newly discovered hybrid boron nitride-carbon nanotubes (BN-CNTs) are very promising for the innovative design of next-generation nanocomposites. In this work, molecular dynamics simulation-based pull-out studies have been performed to characterise the interfacial properties of BN-CNT reinforced polyethylene (PE) composites. Our results show that the interfacial shear strength (ISS) of BN-CNT/PE nanocomposites strongly depends on the BN composition and the connecting pattern of the C/BN fragment in the embedded BN-CNTs. Specifically, an ISS about 90% greater than that of the PE composite reinforced by the conventional carbon nanotube (CNT) is detected in the composite reinforced by the BN-CNT with certain connecting pattern and BN concentration. Such a superior ISS in the BN-CNT/PE composites is found to mainly originate from the unique rough van der Waals surface of the BN-CNT and the greater binding interaction between the embedded BN-CNT and the PE matrix, both of which contribute to enhancing the interface load transfer of nanocomposites. The enhanced ISS detected in the composite reinforced by BN-CNTs suggests that, compared with the most commonly used CNT, the novel BN-CNT can be a better reinforcement candidate in the design of nanocomposites.

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1. Introduction

The discovery of carbon nanotubes (CNTs) has triggered great scientific and engineering interest in the field of one-dimensional (1D) tubular nanomaterials. Besides CNTs, nanotubes of other materials have been studied experimentally and theoretically recently, among which boron nitride nanotubes (BNNTs) have attracted special attention [1–3]. It is proven that both CNTs and BNNTs have exceptional mechanical properties [3,4]. For example, the Young's modulus of both CNTs and BNNTs was experimentally measured and estimated to be in the order of 1 TPa [5,6]. The large Young's

modulus and stiffness of CNTs and BNNTs were also detected in theoretical studies [7,8]. Owing to their remarkable mechanical properties, CNTs and BNNTs can be introduced as promising reinforcement materials for manufacturing lightweight polymeric composite materials. Indeed, significant enhancements in the elastic modulus and strength of polymer composites with an addition of small amounts of 1D tubular nanomaterials have been observed in some recent experiments and simulations [9,10].

In contrast to their mechanical properties, the electronic properties of CNTs and BNNTs are vastly different. CNTs can be metallic or semiconducting depending on the tube chirality and morphology [11], while all BNNTs are permanent semiconductors [12]. In the past decade, many efforts have been made in exploring the combinations of these component materials in order to develop novel hybrid boron nitride-carbon nanotubes (BN-CNTs) with adjustable

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electronic properties [13–15]. Generally, BN-CNTs can be treated as the doping of BN segments into different CNT segments with a suitable formation proportion [16,17]. Theoretical studies show that the electronic properties of BN-CNTs can be tailored by adjusting their forming pattern or BN concentration [18]. In addition, our recent studies [19,20] prove that the Young's modulus and stiffness of BN-CNTs are between those of pristine CNTs and BNNTs. In other words, the mechanical properties (Young's modulus and strength) of BN-CNTs are comparable to those of their pristine CNT and BNNT counterparts (see Ref. [20]). Similar to their CNT and BNNT counterparts, the superior mechanical properties of BN-CNTs to some extent suggest that the BN-CNT can also be an ideal material candidate to serve as the reinforcing agents in nanocomposites. Motivated by this idea, it is of great interest to quantify the mechanical properties of the nanocomposites reinforced by BN-CNTs. Specifically, it is known that the effective load transfer at the interface between the embedded nanofiller and the surrounding polymer matrix is an important design parameter to maximize the contribution of the polymer adsorption layer [21–29]. Thus, the interface load transfer ability of the nanocomposites, which is characterised by the interfacial shear strength (ISS), is critical for the mechanical properties of the nanocomposites [21–29].

In this paper, we use molecular dynamics (MD) simulations to investigate the ISS of the BN-CNT reinforced nanocomposites through the pull-out test, in which an external load is applied on the embedded BN-CNT to pull the nanotube out from the polymer matrix. This pull-out technique has been widely utilized in previous experiments and simulations to measure the ISS of CNT and BNNT reinforced polymer composites [21–29]. In the present pull-out studies, a superior ISS is detected in composites reinforced by the BN-CNT with certain connecting pattern and molar fraction of BN atoms. Some efforts are also made to reveal the mechanism of the enhanced ISS observed in the present BN-CNT/PE composites.

2. Simulation method

In the present study, we considered a (8, 0) zigzag BN-CNT with a helicoidal arrangement of the BN and C stripes (see Fig. 1a). To form this hybrid structure, the C or BN hexagons at the boundaries of the BN and C stripes were doped by one 'impurity' atom (see Fig. 1a). BN-CNTs with this forming pattern were motivated by the existence of helical wrapping patterns in composite nanotube systems [30] and have been proven to be energetically favourable by previous theoretical studies [16,17,30]. The composition of these BN-CNTs was represented by the molar fraction of BN atoms c , which was taken as the ratio of the number of BN atoms to the total number of atoms in the BN-CNT system. As for the matrix, we chose the polyethylene (PE) as an example (see Fig. 1a). The PE, a chain containing 20 monomers $-\text{CH}_2-\text{CH}_2-$, was chosen as the matrix here because its structural simplicity can effectively reduce the computational cost. Moreover, as a representative polymer matrix, PE can give a general picture of the possible interfacial behaviours of various other nanotube/polymer nanocomposites.

In this study, classical MD simulations were adopted to perform the pull-out test on the BN-CNT reinforced PE nanocomposites, which contain three distinct components: BN-CNT, polymer matrix (PE) and interface. In the MD model the atoms are usually treated as point-like masses that interact with one another according to a given potential energy. In the present simulation, the hybrid adaptive interactive reactive empirical bond order (AIREBO)-Tersoff potential was used to describe the BN-CNT. Specifically, the interactions between C atoms of the BN-CNT were described by the AIREBO potential, while the B-N, C-B and C-N interactions were described by the Tersoff potential. The values of the parameters in this hybrid AIREBO-Tersoff potential were taken from Refs. [31–33]

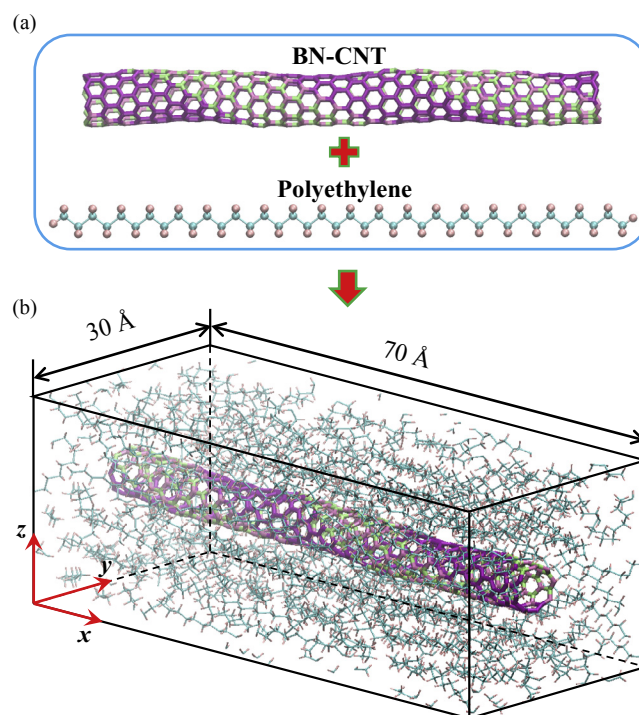


Fig. 1. (a) The molecular structure of a single PE chain and a (8, 0) BN-CNT. (b) Equilibrated structure of the simulation cell for the BN-CNT/PE nanocomposites.

and have been widely used to reveal the optimal morphology of hybrid BN-CNTs [34] and BN-C nanosheets [35]. The PE chains were described by the modified AMBER potential function [22]. The parameters of the AMBER potential function used for the PE were taken from Ref. [22]. The nonbonded van der Waals (vdW) interfacial interaction between the BN-CNT and the PE matrix was modelled by the 12-6 Lennard-Jones (LJ) potential. The parameters of the LJ potential used in the present study were calculated based on Lorentz-Berthelot mixing rules [36] together with the LJ coefficients for C, H, B and N atoms in Refs. [37,38].

In the present simulation, a BN-CNT with a length L of ~ 70 Å was initially created using the lattice constant of CNTs, and then relaxed to a local minimum energy state using the conjugate gradient algorithm. Subsequently, the obtained BN-CNT was placed in the centre of a model box. Meanwhile, 59 PE chains were placed into the model box randomly using the Packmol software [39]. Since Packmol treats molecules as rigid bodies, the size of the model box was initially enlarged to accommodate all PE chains and the BN-CNT. To increase the density of the PE matrix to an experimentally measured value of 0.92 g/cm³ [40], the conjugate gradient method was adopted to compress the model box gradually from its initial dimension to the targeted size of 30 Å \times 30 Å \times 70 Å (see Fig. 1b). After the volume reduction, to distribute the molecules evenly, the compressed box was then equilibrated for 2 ns with the time step 1 fs in the isothermal-isobaric (NPT) ensemble at the temperature of 300 K and pressure of 1 atm. The Nosé-Hoover thermostat algorithm [41] was implemented in this equilibration process. The obtained equilibrated structure of the representative volume element of the BN-CNT reinforced PE nanocomposites was thus ready for the pull-out test. The pull-out simulations of the BN-CNT from the PE matrix were implemented by moving the atoms at the right end of the BN-CNT along the x direction (see Fig. 2a). To reach this goal, the outermost atoms at the right end of the BN-CNT were frozen to maintain the quasi-static pull-out process by a step-by-step movement of these outermost atoms. At the same time, in

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