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Enhanced torsional stability of carbon nanotubes with tensile pre-strain

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HIGHLIGHTS

- Tensile pre-strains greatly enhance the torsional stability of carbon nanotubes.
- Increase rates of buckling torques are in proportion to the degrees of tensile pre-strains.
- Increase rates of buckling torques are much larger in zigzag carbon nanotubes.
- Maximum increase rate of buckling torque is 122.3% in zigzag carbon nanotubes.
- Tensile pre-strains also alter the torsional stiffness of carbon nanotubes.

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ABSTRACT

This work examines the torsional mechanical properties of single-walled carbon nanotubes with tensile pre-strains using classical molecular dynamics simulations. In particular, it is investigated how much the tensile pre-strains enhance the torsional stability of nanotubes, and how this enhanced torsional stability is dependent on the chirality of nanotubes. The observations reveal that the tensile pre-strains greatly enhance the torsional stability of nanotubes and the effects are strongly dependent on the degrees of tensile pre-strains and the chirality of nanotubes. The increase rates of torsional buckling moments are in proportion to the degrees of tensile pre-strains and much larger in zigzag nanotubes than in armchair nanotubes. In the case of zigzag nanotubes, the maximum increase rate of torsional buckling moment is 122.3% for the tensile pre-strain of 0.115. In addition, the tensile pre-strains also alter the torsional stiffness of nanotubes depending on the degrees of tensile pre-strains and the chirality of nanotubes.

1. Introduction

Carbon nanotubes (CNTs) have unique electrical and mechanical properties. They have consequently been proposed for use as key elements in applications such as nanometer-scale electromechanical devices [1–4], biomedical devices [5,6], and composite materials [7,8]. In these CNT-based applications, torsional moments (or torques) are expected to occur widely on the CNTs. For instance, CNTs have been typically incorporated as torsion springs in torsional nanometer-scale devices [9,10]. Therefore, characterizing and understanding the torsional mechanical properties of CNTs are important to optimize their use in new devices and materials.

It has been previously shown that a tensile pre-strain (ε_{tp}) is used in some engineering applications such as piezoelectric actuators [11,12]. In particular, this tensile pre-strain might be also applicable to CNTs incorporated in nanometer-scale devices [13] and materials [14]. For example, the tensile pre-strained CNTs could be used as torsion springs which are doubly clamped-suspended between anchor elements in torsional actuators and oscillators [1,4]. The tensile pre-strain could be induced to CNTs during fabrication or within experimental setups [15]. The tensile pre-strain indicates a preexisting strain before external loads are applied, and can affect the torsional mechanical properties of objects including CNTs [16]. Some studies have shown that the effect of tensile pre-strain on torsional mechanical properties is most important for hyper-elastic materials such as natural rubbers [17] and biomaterials [18] due to their substantial-large tensile elongation features. CNTs also have the hyper-elastic ability to endure relatively large tensile elongation [19–21]. It is therefore expected that the tensile pre-strain is also able to influence significantly the torsional mechanical properties of CNTs. Consequently, exploring the effect of tensile pre-strain on the torsional mechanical

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properties of CNTs would be also very helpful to optimize the use of tensile pre-strained CNTs in new torsional devices and materials. While numerous studies have examined some aspects of the torsional mechanical properties of CNTs under uniaxial [22–29] and simultaneously combined loading [30–36], there is much that is still unknown about other aspects of the torsional mechanical properties of tensile pre-strained CNTs, especially concerning the chirality dependence on their enhanced torsional stability.

This work examines the torsional mechanical properties of single-walled carbon nanotubes (SWCNTs) with tensile pre-strains using classical molecular dynamics (MD) simulations. In particular, it is carefully investigated how much the tensile pre-strains enhance the torsional stability of CNTs, and how this enhanced torsional stability is dependent on the chirality of CNTs. To our best knowledge, the results have not been presented previously and are expected to provide new insights that will enhance the design of nanometer-scale devices and composite materials based on CNTs.

2. Methods

The classical MD simulations numerically integrate Newton's equations of motion with a third-order Nordsieck predictor corrector using a time-step of 0.2 fs [37]. The forces on the atoms are calculated using methods that vary with interatomic distance. In particular, the short-range covalent interactions are modeled using the many-body, second generation reactive empirical bond-order (REBO) hydrocarbon potential [38]. It has been previously demonstrated that the cutoff functions of the REBO potential overestimate the force needed to break a carbon–carbon covalent bond [20]. In order to prevent this overestimation, we have used the modified cutoff function for distances between 1.7 and 2.0 Å in the same way as the literature which was previously published [20]. In addition, long-range van der Waals interactions are included in the form of a Lennard-Jones potential [37]. The system temperature is maintained at 300 K using a velocity-rescaling thermostat that has been shown to have negligible effects on the mechanical behavior of CNTs [39]. The particular nanotubes that are considered are (15,15) armchair and (26,0) zigzag SWCNTs. The nanotubes are about 9.5 nm long, and only defect-free nanotubes are considered here.

The tensile pre-loads are applied to one ends of undeformed CNTs (reference configuration) while their other ends are held fixed to achieve the tensile pre-strained CNTs. The degrees of tensile pre-strains that are considered are shown in Table 1 and much lower than the values of tensile failure strains. The torsional moments are then applied to one ends of the tensile pre-strained CNTs while their other ends are held fixed. Hence, both ends of the tensile pre-strained CNTs are fixed in the axial direction to keep the tensile pre-strains balanced. This simulation setup is also identical to the conditions of torsional devices based on CNTs [1–4], so that Poynting effect is not considered in this work [40]. It should be especially notified that the MD simulations are based on the quasi-static and load-control method. In these MD simulations, the applied loads are incremented quasi-statically to the nanotubes, and then their displacements are obtained during the simulations. Therefore, this approach is similar to the quasi-static testing of macroscopic materials and structures that especially adopts the load-control method. The applied tensile and torsional loading rates during MD simulations correspond to deformation rates of 10 m/s and 10 grad/s, respectively. These loading rates are low enough to avoid adverse effects on the mechanical behaviors of CNTs.

Table 1
The degrees of tensile pre-strains that are considered to achieve the tensile pre-strained CNTs. The values of given tensile pre-strains are much lower than those of tensile failure strains. These tensile pre-strains are applied identically for (15,15) armchair and (26,0) zigzag SWCNTs.

Type	Tensile pre-strain
P1	0.018
P2	0.038
P3	0.060
P4	0.115

3. Results and discussion

While CNTs have high rigidity along their tensile direction, they are compliant in their radial direction due to tubular shape [41–46] and the absence of inner materials. Therefore, the failure behavior of CNTs under loads such as torsional moments reveals instability (or buckling) as illustrated in Fig. 1. When the torsional moments are applied to the CNTs, the nanotubes are rapidly contracted in their radial direction after the buckling onset due to the absence of inner materials, so that constant torsional moments are sufficient to further deform the nanotubes and their buckled configurations exhibit substantial kinks [23]. Consequently, the effective torsional stiffness is decreased to nearly zero after the buckling onset, indicating torsional instability as shown in Fig. 1. This torsional instability has been known to be influenced by the chirality of CNTs [22]. Fig. 1 demonstrates the chirality-dependent torsional instability in the cases of (15,15) armchair and (26,0) zigzag SWCNTs under pure torque (without tensile pre-strain). In the figure, we can see that the torsional buckling moment for (15,15) armchair SWCNTs is slightly larger than that for (26,0) zigzag SWCNTs. This result is in good agreement with previously published predictions [22]. However, the torsional stiffness is not greatly affected by the chirality of CNTs, as indicated in Fig. 1.

As mentioned earlier, it is expected that the tensile pre-strain is able to influence the torsional mechanical properties of CNTs due to the coupling effects with the tensile pre-strain. Fig. 2 presents the coupling effects of tensile pre-strain on the torsional behavior of (15,15) armchair SWCNTs in terms of a torsional angle. The figure illustrates that the torsional buckling moments significantly increase in proportion to the degree of tensile pre-strain (see Table 1). In the other word, the figure indicates that the torsional stability of CNTs is greatly enhanced by the tensile pre-strain and the effect is strongly dependent on the degree of tensile pre-strain. This is because the torsional instability of CNTs is restricted by the tensile pre-strain preexisting on them. In addition, the figure also

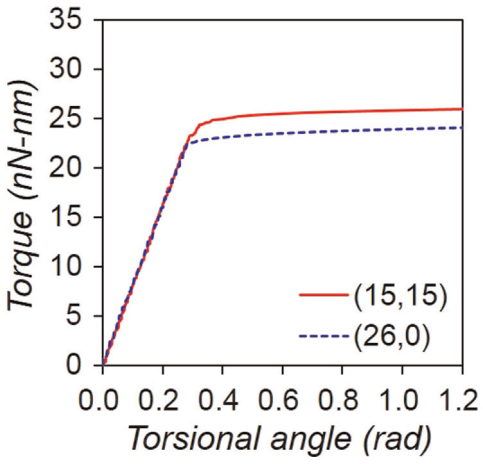

Fig. 1. Torsional behaviors of (15,15) armchair and (26,0) zigzag SWCNTs under pure torques. Tensile pre-strains are not applied in the condition of pure torques.