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Tension–twisting dependent kinematics of chiral CNTs

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ABSTRACT

This paper shows that chiral carbon nanotubes (CNTs) under twisting show highly dependent strength and fracture toughness on (i) the level of axial tension and (ii) the direction of twisting. To achieve this conclusion, numerous computational intensive molecular dynamics simulations of chiral (6,3) CNTs were performed using the LAMMPS code and the AIREBO potential for C–C bonds. First, we have studied the influence of the tension level and the direction of twisting on the buckling and failure of the chiral CNTs. We show that the applied torques and angles of twist at the buckling and failure stages strongly depend on the level of tensile loading and on the twist direction. In order to explain such noticeable anisotropic behaviour, we have studied the evolution of two kinematic variables (C–C bond length and hexagonal cell angle) as a function of the twist–tension rate. We conclude that the anisotropic failure of chiral CNTs strongly depends on the type of rupture mechanism, which varies with (i) the level of axial tension and (ii) the direction of twisting. Finally, we summarize the information by means of tension–twisting interaction diagrams, which are very dissimilar for direct and inverse twisting. We conclude that inverse twisting influences very negatively the collapse behaviour of chiral CNTs under tension. On the other hand, for low-to-moderate twist–tension rates, the coupling between tension and direct twisting is highly beneficial for the behaviour of chiral CNTs against collapse. This scenario changes dramatically for moderate-to-high twist–tension rates, as the coupling between tension and direct twisting becomes highly detrimental for the chiral CNT collapse process. These original findings might be relevant for the design of nano-devices made of chiral CNTs, as we show that the fracture toughness of chiral CNTs under tension can be highly increased if low-to-moderate direct twisting is added.

1. Introduction

The use of carbon nanotubes (CNTs) in nano-devices (nano-drive systems, nano-actuators, nano-oscillators), for instance as spring elements in torsional paddle oscillators or twisting bearings in nano-electric motors, as prompted a lot of research on their mechanical behaviour under different directional loads. This research can be accomplished with either experiments or molecular dynamics (MD) simulations. Owing to the complexity in setting up rigorous test arrangements to make measurements at the nanoscale, experimental investigations are scarce [1]. On the other hand, MD simulations have been widely used to study the mechanical behaviour of CNTs. Both the pure axial (tensile and compressive) and the pure twisting mechanical behaviours of armchair, zigzag and chiral CNTs were investigated (e.g. [2–5]). Nevertheless, pure loading actions are difficult to occur at nanoscale level due to support imperfections, load eccentricities and geometrical inaccuracies of fixing nanotubes in nano-devices. Thus, combinations of individual (pure) loadings are expected to take place and understanding the CNTs mechanical response to combined loading is crucial to the design and optimization of CNT-based devices. Regarding the use of MD to simulate CNTs under combined tension–twisting, few works have been published [6–8]. Jeong et al. [6] concluded that armchair and zigzag CNTs under combined tension–twisting have decreasing tensile strength with linearly increasing twist. Talukdar and Mitra [7] concluded that the defects change significantly the mechanical properties of armchair CNTs as well as their failure stresses and failure strains. Jeong et al. [8] developed failure criteria for the strength of armchair CNTs under tension–twisting and indicated that yielding or fracture behaviour of CNTs "*should be described by detailed atomistic observations involving chemical bond breaking, and therefore cannot be described with only macroscopic or continuum modeling that lack these atomistic details*". This is the main reason for using MD simulations in the present study, instead of either molecular mechanics or continuum models. In a recent paper [9], the authors unveiled the twist-induced elastic anisotropic behaviour of chiral CNTs under pure twisting and moderate-to-high twist–tension rate. We showed

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that the addition of axial tension plays a key role in the chiral CNT linear and post-buckling stiffness. However, we did not attempt to study the continuous evolution of (i) chiral CNTs strength and fracture toughness and (ii) the type of failure mechanism, under different twist–tension rate regimes (either low, moderate or high). The present paper investigates the above mentioned issues, as well as the tension–twist interaction diagrams at failure, using MD simulations.

2. Scope and parameters of MD

Molecular dynamics (MD) simulations were performed using the Large Scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) code [10]. The C–C interaction parameters follow the latest version of the AIREBO potential proposed by Stuart et al. [11]. The AIREBO potential is an improved version of Brenner's well-known second generation Reactive Empirical Bond Order Potential (REBO) but includes a Lennard-Jones potential form to describe van der Waals long-range interactions and a torsional term for σ-bond torsions. It has been previously demonstrated that the cutoff functions of the Brenner, REBO and AIREBO potentials overestimate the force needed to break a carbon–carbon covalent bond [6,12–14]. Recently, Kim et al. [14] performed a study on graphene failure and showed that no C-chains pull out when ReaxFF potential is used (instead of AIREBO), which may be due to smoother cutoff. In AIREBO potential, the cutoff function introduces a high increase in the interatomic force at the minimum distance, like a "camelback" on the force curve [12]. The influence of cutoff functions is mostly felt for CNTs under tensile loading rather than compression, twisting or bending. Following previous works, we adopted cutoff distances of 1.7 Å (minimum) and 2.0 Å (maximum). In this work we have considered only chiral CNTs ($n = 6$, $m = 3$) with radius $R = 3.1$ Å, chiral angle $\theta = 21.2°$, length $L = 41.0$ Å, aspect ratio $L/D = 6.6$ and 336 C-atoms. A more detailed explanation on the incremental loading procedure can be found in [15]. The combined twist–tension loading is imposed using a similar procedure to that described by Faria et al. [15] – see Fig. 1 in [15]. In the present study, tensile loading is applied to the CNT by moving the top and bottom boundaries apart in the axial direction using prescribed increments, while in [15] compressive loading was applied to the CNT by moving these boundaries closer. The CNTs chirality provides two distinct directions of twist: direct twisting and inverse twisting – see Fig. 1. Direct twisting corresponds to rotating both ends of the CNT in opposite directions following the rolling of the hexagon lattice (image in the left side of Fig. 1a) while inverse twisting corresponds to rotating both CNT ends in opposite directions but opposing the rolling of the hexagonal lattice (image in the right side of Fig. 1a). For combined twist–tension, both loadings are applied simultaneously. For a given combination, a twist-to-tension rate $\Delta\phi/\Delta u$ is defined, which means that the CNT twists $\Delta\phi/\Delta u$ radians (rad) for each Ångstrom (Å) of stretching. In order to better present the results, the twist-to-tension rate $\Delta\phi/\Delta u$ can be transformed into an angle β given by $\beta = \tan^{-1}\left(\frac{\Delta\phi}{\Delta u} \times \frac{\Delta u_0}{\Delta\phi_0}\right)$, where $\Delta u_0 = 0.050$ Å and $\Delta\phi_0 = 1.0° = \pi/180$ rad are the displacement and twist rotation imposed in each increment. The results are presented and discussed next.

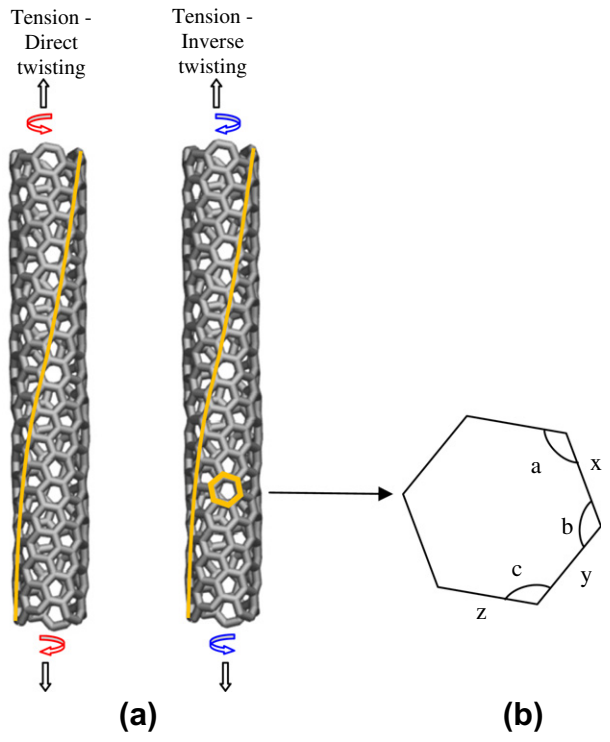

Fig. 1. (a) A (6,3) chiral CNT under direct and inverse twisting and (b) labeling of bonds and angles in a hexagonal cell (the yellow line denotes the orientation of the zig–zag line that spirals around the CNT in the initial non-deformed state).

3. Influence of twist-to-tension ratio

Figs. 2 and 3 show the variation of the torque T with the angle of twist ϕ, for direct and inverse twisting, respectively. The torque corresponds to the first derivative of the energy w.r.t. the angle of twist ($T = \partial V/\partial\phi$). Three twist-to-tension rates are considered: $\Delta\phi/\Delta u = 0.349$ rad/Å ($\beta = 45°$ – [1]red curve), $\Delta\phi/\Delta u = 0.605$ rad/Å ($\beta = 60°$ – blue curve), and $\Delta\phi/\Delta u \to \infty$($\beta = 90°$ – black curve). Note that the $\beta = 90°$ curve corresponds to pure twisting (i.e., no tension).

The observation of Fig. 2 (direct twisting) enables the following remarks:

- The torque varies significantly with the twist-to-tension rate. Regardless of β, there is always an initial linear ascending path followed by a linear but less ascending path. In the initial path the shape of the CNT remains cylindrical while in the second path it assumes a helix shape [16]. The transition point between the two paths is called a bifurcation point (circle) and the corresponding torque is designated as critical torque T_c.
- The slope of these paths and the critical torque T_c increases with decreasing β. This fact means that tensile loading stiffens the CNT: it is more difficult to twist the tensioned CNT ($\beta = 45°$ and $\beta = 60°$) than the CNT free of tension ($\beta = 90°$).
- The second path achieves a maximum torque (circle), designated as failure torque T_f, after which it suddenly drops. The failure torque T_f also increases with decreasing β. This evidence also means that tensile loading strengthens the CNT: the failure torque is higher for the tensioned CNT ($\beta = 45°$ and $\beta = 60°$) than for the CNT free of tension ($\beta = 90°$).
- Regarding the mechanical behaviour of CNTs, we propose here two important measures: the strength factor $\eta = \frac{T_f}{T_c}$ and the ductility factor $\chi = \frac{\phi_f}{\phi_c}$. The strength factor measures the CNT ability to resist loads without collapsing while the ductility factor measures the CNT capacity to deform without collapsing. From MD data, we got $\eta = 1.56$ and $\chi = 2.61$ ($\beta = 45°$), $\eta = 1.76$ and $\chi = 3.01$ ($\beta = 60°$), $\eta = 1.83$ and $\chi = 10.34$ ($\beta = 90°$). These results mean that the strength factor slightly increases with the twist-to-tension rate. This is also the case of ductility factor for low-to-moderate twist-to-tension rate ($45° \leqslant \beta \leqslant 60°$). Surprisingly,

[1] For interpretation of color in Figs. 1–7, 9 the reader is referred to the web version of this article.