Mechanics Research Communications 73 (2016) 19–24

Contents lists available at ScienceDirect

Mechanics Research Communications

journal homepage: www.elsevier.com/locate/mechrescom

Mechanical behaviour of carbon nanotubes under combined twisting–bending

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ARTICLE INFO

Article history:
Received 1 September 2015
Received in revised form
30 November 2015
Accepted 26 January 2016
Available online 4 February 2016

Keywords:
Carbon nanotube
Mechanical behaviour
Twisting–bending
Failure
Buckling

ABSTRACT

The main objective of this paper is to investigate the mechanical behaviour (strength and stiffness) of carbon nanotubes (CNTs) under combinations of bending and twisting. In order to achieve this goal, molecular dynamics (MD) simulations of bended and twisted CNTs are performed. The LAMMPS code is used, the AIREBO potential is considered for C—C bonds, the temperature is kept at 300 K and incremental bending and twisting rotations are imposed to the CNT. Two types of CNTs are analyzed, including zig-zag (8,0) and armchair (5,5) CNTs with similar radius and length. The CNTs are also analyzed for pure bending and pure twisting. The main results are shown in the form of diagrams of energy and moment against imposed rotations. Some relevant conclusions are drawn concerning the influence of loading (bending and twisting) on the stiffness, strength and failure of CNTs: namely, it is concluded that armchair CNTs possess higher strength and fracture toughness under twisting–bending loading than zigzag CNTs; additionally, it is found that both CNTs (armchair and zigzag) still support moderate-to-high bending levels without failure after being extremely twisted and torsionally buckled, even for twisting angles four times those corresponding to torsional buckling; finally, the results prove that CNTs, mostly armchair ones, exhibit very high twisting–bending stiffness and strength and can be used with confidence as torsional spring elements in nanoelectromechanical systems (NEMS).

1. Introduction

Due to their exceptional mechanical properties, carbon nanotubes (CNT) have been used not only for reinforcement of materials in novel nanocomposites but also for building blocks in the design of nano-devices such as nano-drive systems, nano-actuators and nano-oscillators. The prediction of the mechanical behaviour of CNTs subjected to different directional loads, simultaneously or not, is a key-factor for optimum design of next generation CNT-based materials and nanodevices. Computational methods, in particular molecular dynamics (MD), have been widely used to study the mechanical behaviour of CNTs. Research works addressing the strength and buckling of CNTs subjected to unidirectional (individual) loads, such as twisting, bending, tension and compression, have been published and are comprehensive [1–3].

Concerning pure bending deformations it is well known that CNTs form a kink for bending angles higher than their critical bending angle. After the formation of this kink, 5–7 Stone-Walls defects emerge [4]. Tang et al. [5] pointed that kink formation may be useful if controlled bending is applied because, when the kink forms, the CNT sidewalls are compressed. This compression pushes carbon atoms together enabling the formation of new carbon–carbon bonds with sp^3 hibridization, increasing the reactivity on the bended surface of the walls. In this way, bending deformations constitute a valid mechanism for controlling functionalization reactions on a CNT. Mylvaganam et al. [6] found the critical bending angle for zig-zag CNTs with small length-to-diameter ratio (~5,5) to be around 24° and showed that the strain energy has a quadratic increase until the formation of the kink. On a broader study, Cao and Chen [7] demonstrated that the critical bending curvature decreases inversely to the square of the tube diameter and they stated that these results are not sensitive to the chirality of the CNT.

Concerning pure twisting deformations, it is known that CNTs buckle in uniform helix deflected shapes. Since the work of Clauss et al. [8], it is known that CNTs under torsion are prone to the distortion of the sp^2-bonded structure and also to the deformation of the tube itself. More recently, Giusca et al. [9] used spectroscopy to characterize the atomic and the electronic structure of a twisted CNT. These works demonstrated the influence of twisting and torsional buckling of CNTs on their electronic properties. Due to the

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http://dx.doi.org/10.1016/j.mechrescom.2016.01.010
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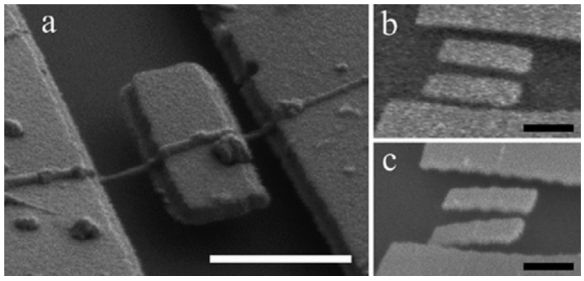

Fig. 1. Single-paddle torsional oscillator with CNT spring element; the CNT is subjected not only to twisting uniformly distributed along its length but also to bending due to paddle self-weight.
(Image taken from [22], with permission of American Physical Society).

fact that torsional buckling of CNTs also erodes their mechanical properties, several investigations have also been devoted to study the mechanical behaviour of CNTs under pure twisting [10–17].

However, due to misalignments, imperfections and eccentricities, the case of CNTs subjected to pure loading (compression, bending, torsion) is more the exception than the rule. Nevertheless, CNTs subjected to combined loading, which is expected to occur in several CNT applications in nanodevices, has been addressed by only a few authors, mostly focusing on tensile-twisting deformations [18]. As an example, CNTs are being used as torsional springs in paddle oscillators (see Fig. 1 [22]) and other nanoelectromechanical systems (NEMS), in which they are twisted and bended. Regarding the behaviour of CNTs under combined loading, the authors have developed comprehensive work by studying in previous works the stiffness and strength of CNTs under compression-twisting [19] and tension-twisting [20,21]. In this paper, we address the mechanical behaviour of CNTs under combined twisting–bending. Using MD simulations, bending deformations are applied to pre-twisted CNTs with similar geometry (aspect ratio) but displaying two different chiralities. The deformation energy and bending moment variation with the imposed rotation (bending and twisting) are presented. These results clarify the influence of twisting on the critical bending angle of CNTs. To the authors' knowledge, the present paper is the first MD study on bending of pre-twisted CNTs.

2. MD simulations and loading procedure

Molecular dynamics (MD) simulations were performed using the Large Scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) [23]. The C–C interaction parameters follow the latest version of the AIREBO potential proposed by Stuart et al. [24] and included in the LAMMPS software package. 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 the Van-der-Waals long-range interactions and an additional term for the σ-bond torsional stiffness. In order to avoid geometry dependent effects, two CNTs with similar aspect ratio L/D are considered, differing only in their chirality:

- The ($n = 8, m = 0$) *zigzag* CNT with radius $R = 3.1$ Å, length $L = 46.3$ Å, aspect ratio $L/D = 7.4$ and 352 C-atoms;
- The ($n = 5$, $m = 5$) *armchair* CNT with radius $R = 3.4$ Å, length $L = 47.3$ Å, aspect ratio $L/D = 7$ and 380 C-atoms;

The combined loading procedure comprised two main steps. In the first step, the CNT was twisted by rotating both ends in opposite directions (see Fig. 2(a)). An incremental displacement $\Delta\phi R$ in the circumferential direction was imposed to the atoms at the CNT

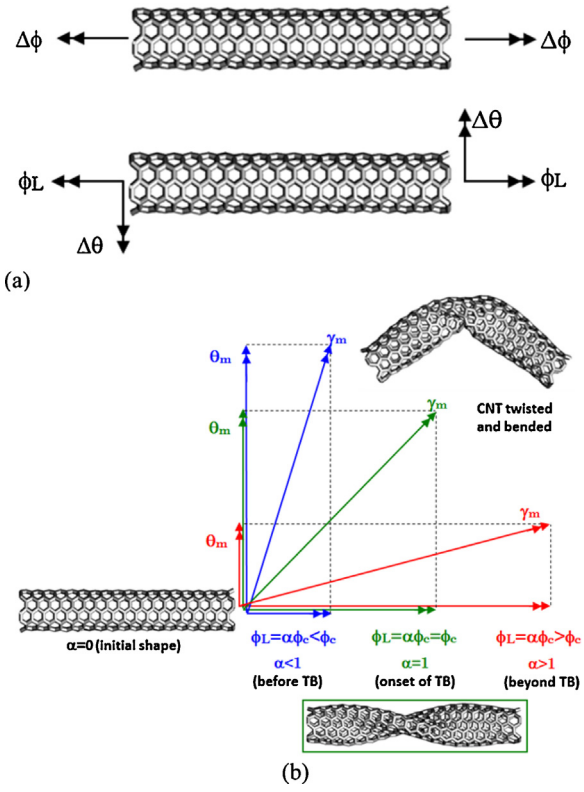

Fig. 2. (a) 1st step of MD (incremental twisting) and 2nd step of MD (incremental bending), (b) possible cases (A, B, C) of CNT under twisting–bending combination.

boundaries (left and right CNT edges rotate $\Delta\phi$ in opposite directions). Therefore, an incremental twisting angle $2\Delta\phi$ was imposed to the CNT. This loading method is identical to the one proposed for pure twisting loads by Faria et al. [19–21]. The first step ends when the angle of twist reaches a limit value ϕ_L. After the first step, the CNT may be in one of three situations:

- Case A – the CNT is twisted but not buckled, meaning that the limit angle of twist ϕ_L is lower than the critical angle of twist ϕ_c. The CNT is in torsional pre-buckling state.
- Case B – the CNT is twisted and buckling occurs precisely for the limit angle of twist ϕ_L, meaning that ϕ_L is equal to the critical angle of twist ϕ_c. The CNT is at the onset of torsional buckling.
- Case C – the CNT is twisted and buckled, meaning that the limit angle of twist ϕ_L is higher than the critical angle of twist ϕ_c. The CNT is in torsional post-buckling state.

In the second step of the procedure, the twisted CNT was bent. At the limit twisting angle ϕ_L, the twist was paused (kept fixed) and incremental bending angles $\Delta\theta$ are imposed to the CNT (see Fig. 2(b)). Both ends of the CNT initiate a rotation about the axis perpendicular to the CNT centroidal axis, causing symmetrical bending of the CNT. Then, bending of CNT was increased (augmenting θ) till the CNT failed by twisting–bending and collapse occurred for a maximum value of bending angle θ_m and prescribed limit value of twisting angle ϕ_L (see Fig. 2(c)). It is possible to sum geometrically both rotation vectors (ϕ_L and θ) and obtain the overall rotation of the CNT boundaries in each increment, $\gamma = \sqrt{\phi_L^2 + \theta^2}$ and also the overall rotation at failure $\gamma_m = \sqrt{\phi_L^2 + \theta_m^2}$ (see Fig. 2(c)).

In the first step of each simulation, the atoms located in both boundaries (circular sections) move according to a prescribed increment and then freeze. The remaining steps allow all other atoms to move unrestrainedly for the structure to relax and reach