MECHANICAL BEHAVIOUR OF TENSIONED AND TWISTED CHIRAL CARBON NANOTUBES

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Abstract

It is well known that CNTs are sensitive to compression, bending and torsion, due to their hollow configuration. Concerning the compressive behaviour, it is now well understood that CNTs are prone to both local and global instability. Molecular dynamics (MD) simulations have shown that the buckling behaviour of a given CNT is length dependent and may be divided into two categories: (i) the shell-like instability (local buckling) for short to intermediate length, and (ii) the beam-like instability (global buckling) for moderate to long lengths. For CNTs with short to intermediate length, the critical strain is not sensitive to the length, while for long CNTs the critical strain depends on the length. For a given CNT structure (n,m), it is also clear that there is an aspect ratio value (length over diameter) that separates the range of local instability from the range of global instability. On the other hand, CNTs under torsion are always sensitive to local instability and the critical twist angle always decreases with increasing length [1]. The first objective of this paper is to shed light on the strength and stiffness of chiral CNTs under torsion, but now combined with tension. The second main goal is to investigate the kinematics of bonds between carbon atoms and its evolution with the applied loading. In order to assess the collapse behaviour of chiral CNTs, MD simulations of twisted and tensioned CNTs are performed. The LAMMPS code is used, the Tersoff-Brenner potential is considered for C-C bonds, the temperature is kept in 300 K and the incremental displacements u and rotations θ are imposed in CNT ends. The results are shown in the form of interaction (ε_{ul}-α_{cr}) diagrams, where $\varepsilon_{ul}=u_{ul}/L$ is the ultimate tension strain and $\alpha_{cr}=\phi_{cr}/L$ is the critical angle of twist per unit of length. After that, some relevant conclusions are drawn concerning the most influential loading on the chiral CNT collapse: twisting over strain or strain over twisting. Then, an interaction formula based on analytical expressions of continuum mechanics is proposed and its results are compared with those obtained from MD simulations. After this study, special attention is devoted to the evolution of C-C bond lengths and angles with the applied loading, which explains the distinct mechanical behaviour of chiral CNTs and shed light on the anisotropic constitutive law of chiral CNTs. Finally, it is shown that buckled CNTs stiffness and strength does not cease beyond first buckling.

For illustration purposes, Figure 1 shows a set of four snapshots of the chiral (6,3) CNT under several twist-to-tension ratios: pure tension (1st snapshot), combination A with twist-to-tension ratio $\Delta\phi/\Delta u$=0.349 rad/Å (2nd snapshot), combination B with twist-to-tension ratio $\Delta\phi/\Delta u$=0.605 rad/Å (3rd snapshot), pure twisting (4th snapshot). Figure 1(a) presents the initial (unloaded) configuration of the CNT while Figures 1(b), 1(c), 1(d) and 1(e) present the deformed shapes of the CNTs after 100, 200, 300 and 400 increment, respectively. The Figures in the left side (1(b_1), 1(c_1), 1(d_1), 1(e_1)) involve direct twisting of the CNT while the Figures in the right side (1(b_2), 1(c_2), 1(d_2), 1(e_2)) involve inverse twisting of the CNT. From this Figure, it is observed that the CNT degradation and the evolution of its collapse is totally different if the CNT is under direct or inverse twisting. For combinations A (0.349 rad/Å – 2nd snapshot) and B (0.605 rad/Å – 3rd snapshot), the CNT also behaves differently for direct and inverse twisting – for instance, see the 2nd snapshot in Figures 1(d_1) and (d_2). The tensioned CNT under direct twisting (combination A) tends to buckle into an helix-shape at early stages (200 increments - Figure 1(c_1)) without rupture. A clear rupture is visible only at 400 increments (Figure 1(e_1)). The tensioned CNT under inverse twisting (combination A) does not tend to buckle into an helix-shape and shows a localized rupture at an early stage (200 increments - Figure 1(c_2)). For combination B, a similar behaviour is observed, but the CNT collapse occurs earlier for both direct and inverse twisting.

References

[1] Faria B., Silvestre N., Canongia Lopes J.N. – "Interaction diagrams for carbon nanotubes under combined shortening-twisting", *Composites Science and Technology*, 71 (2011), 1811-1818.

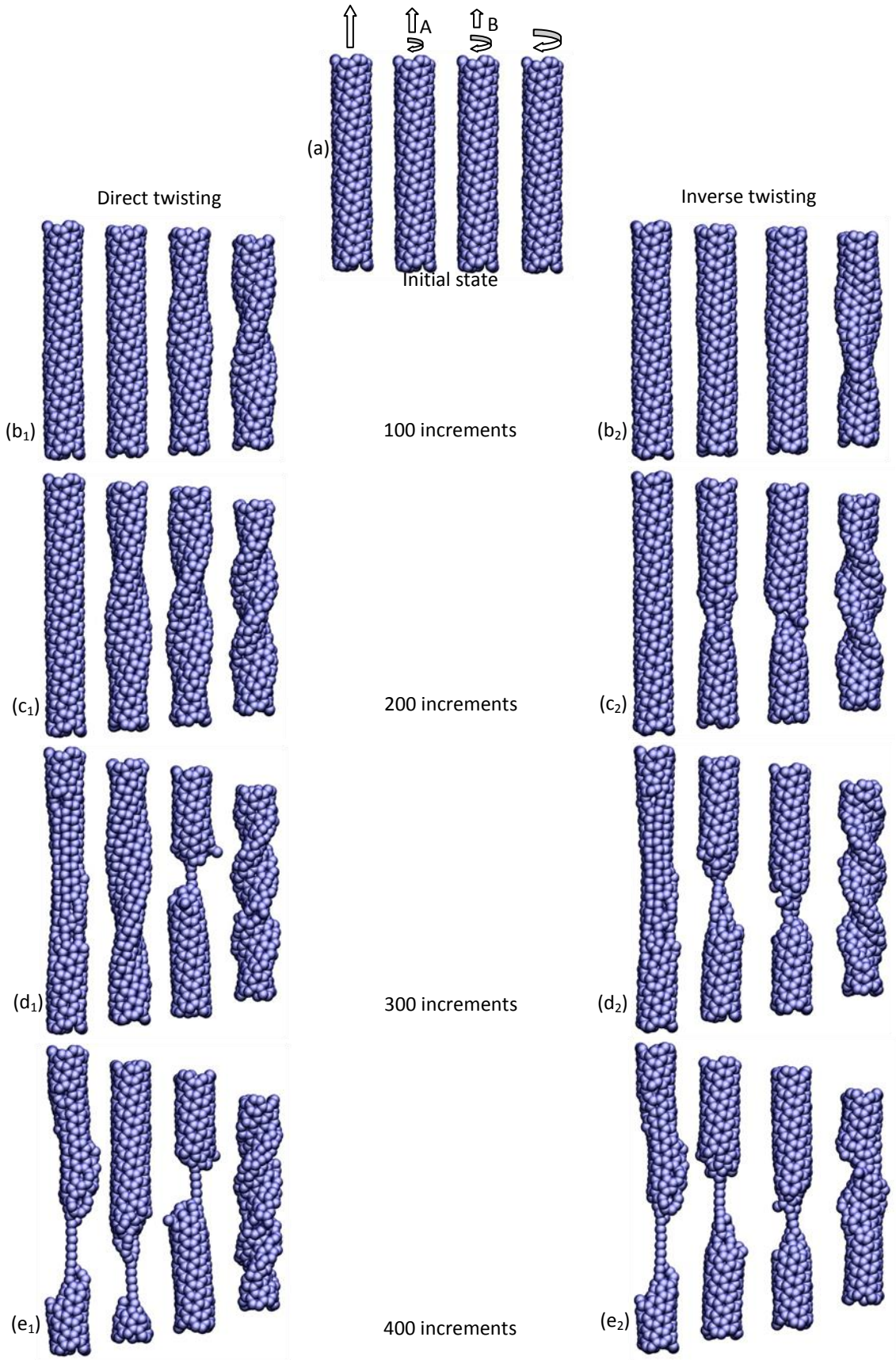

Figure 1: Deformed shapes of the CNT under tension-to-twist rates: (a) initial (unloaded), (b) after 100 increments, (c) after 200 increments, (d) after 300 increments and (e) final (after 400 increments) - (b_1), (c_1), (d_1), (e_1) for direct twisting and (b_2), (c_2), (d_2), (e_2) for inverse twisting.