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MECHANICAL BEHAVIOR OF CARBON NANOTUBES ENCAPSULATING COPPER ATOMS

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In nanoelectromechanical systems (NEMS), torsional devices can be used for a wide number of applications including sensors, signal processors, optical modulators, clocks for electronics, and resonators, etc. Due to their excellent mechanical, electrical, and thermal properties, carbon nanotubes (CNTs) are expected to be the ideal candidate for use as torsional springs in NEMS [1-3]. CNTs can also act as torsional electromechanical oscillators [4] or rotational bearings in actuators [5]. Furthermore, CNTs subjected to torsion can also serve as a channel for transportation of hydrogen molecules [6]. Thus, it is important to gain a clear understanding about the torsional behavior of carbon nanotubes.

The encapsulation of metal atoms into the internal cavity of carbon nanotubes may significantly alter their conducting, electronic and mechanical properties and create intriguing multifunctional nanodevices. Figure 1 shows the initial equilibrium configurations of some metal-filled CNTs. Metal atoms aggregate in a fashion consisting of concentric layers. Filling of metal atoms may alter the torsional behavior of CNTs and hence this topic is investigated in the present work.

Using classical molecular dynamics method, firstly, the induced torsion of single-walled carbon nanotubes filled with copper atoms is investigated under axial tension and compression. Results show that this coupling response between torsional deformation and axial strain is only limited to chiral filled tubes. As compared with the behavior of empty chiral tubes, due to the van der Waals interaction between tube wall and the encapsulated metal atoms, the induced torsional behavior of chial filled tubes is reversed and its diameter dependency is contrary. Secondly, the buckling deformation of single-walled carbon nanotubes completely filled by copper atoms is studied under external torsion. Due to the metal filling, the torsional rigidity of tubes can be dramatically enhanced and the critical torsional angles of filled tubes can be 2~4 times higher than those of empty ones. Furthermore, due to structural asymmetry in chiral metal-filled tubes, there exists a dependency of the torsional behavior on loading directions. These results can provide helpful guidelines for the applications where carbon tubes serve as torsional devices.

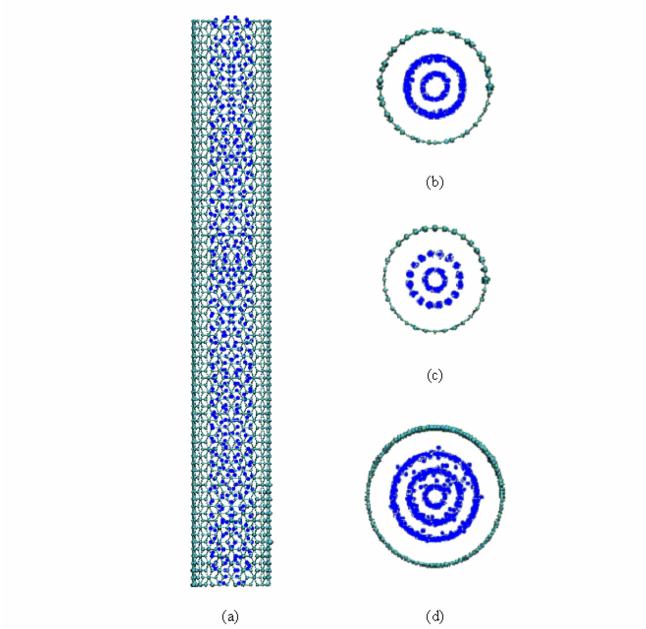

Figure 1. Initial unstrained configurations of metal-filled carbon nanotubes: (a) and (b) are front and top views of (10, 10) armchair tube, while (c) and (d) are top views of (16, 0) zigzag tube and (16, 8) chiral tubes, respectively.

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