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A rod model for three dimensional deformations of single-walled carbon nanotubes

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ABSTRACT

A continuum model for single-walled carbon nanotubes (SWCNT) is presented which is based on an extension to the special Cosserat theory of rods (Kumar and Mukherjee, 2011). The model allows deformation of a nanotube's lateral surface in a one dimensional framework and hence is an efficient substitute to the commonly used two dimensional shell models for nanotubes. The model predicts a new coupling mode in chiral nanotubes – coupling between twist and cross-sectional shrinkage implying that the three deformation modes (extension, twist and cross-sectional shrinkage) are all coupled to each other. Atomistic simulations based on the density functional based tight binding method (DFTB) are performed on a (9,6) SWCNT and the simulation data is used to estimate material parameters of this rod model. A peculiar behavior of the nanotube is observed when it is axially stretched – induced rotation of each cross-section is equal in magnitude but opposite to that of its two neighboring cross-sections. This is shown to be an effect of relative shift/inner-displacement between the two SWCNT sub-lattices.

1. Introduction

Interest in carbon nanotubes has surged in the recent past due to their exceptional mechanical and electrical properties (Yakobson et al., 1996; Gartstein et al., 2003; Dresselhaus et al., 2004; Liu et al., 2004; Sazonova et al., 2004; Liang and Upmanyu, 2006). Now they are being studied extensively for their potential application as fibers (Qian et al., 2000), sensors (Kong et al., 2000), tunable oscillators (Sazonova et al., 2004), synthetic gecko foot-hairs (Yurdumakan et al., 2005), etc. to name a few. An important area of research concerning carbon nanotubes is characterization of their mechanical behavior based on elastic continuum models (Lu, 1997; Govindjee and Sackman, 1999; Sáncez-Portal et al., 1999; Ru, 2000; Arroyo and Belytschko, 2002; Pantano et al., 2003; Chang and Gao, 2003; Wu et al., 2008; Chandraseker et al., 2009). The assumption of elasticity stems from the observation that SWCNTs undergo large, reversible deformations without developing lattice defects (Iijima et al., 1996; Yu, 2004). Such elastic continuum models can be very useful for studying large scale phenomena of atomic systems since they capture collective behavior of atoms and offer computational efficiency by reducing their degrees of freedom. However, in spite of the robustness and economy of continuum models, use of traditional continuum models for CNTs can lead to inconsistencies due to surface, interface, size effects (Yakobson et al., 1996; Bar On et al., 2010) and ambiguities associated with model parameters such as elastic moduli and CNT wall thickness.

Elastic continuum models of CNTs can be broadly classified into one, two and three-dimensional ones. Li and Chou (2004) proposed a three dimensional model of a space truss network for SWCNTs. They took into account all the atoms in a given SWCNT segment without any coarse-graining, and hence the model is computationally very expensive. Two-dimensional continuum models of CNTs have been based on elastic thin-shell models with Young's modulus and wall thickness as input parameters (Pantano et al., 2003, 2004). In the large strain regime, the quasi-continuum approach, proposed originally for bulk crystals (Shenoy et al., 1999; Tadmor et al., 1999), has been used for atomistic-continuum modeling of mechanical deformations of SWCNTs to derive a nonlinearly elastic membrane model (Zhang et al., 2002; Arroyo and Belytschko, 2004; Liu et al., 2004; Chandraseker et al., 2006; Wu et al., 2008; Chang, 2010). Such models have the advantage that they capture material nonlinearity accurately as the material parameters are computed directly from an inter-atomic potential for any given strain level.

At a longer length scale, the deformation of a nanotube's lateral surface becomes less significant and it makes sense to use a one dimensional model for a SWCNT. Indeed, Buehler et al. (2004) show that as the length of a nanotube is increased, the nanotube makes a transition from shell to rod and then finally to a wire at which stage a nanotube can potentially undergo self-folding

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