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In-plane elastic moduli of covalently functionalized single-wall carbon nanotubes

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ABSTRACT

Effective utilization of single-wall carbon nanotubes (SWCNTs) as reinforcements in composites necessitates their strong interfacial bonding with the surrounding matrix. The covalent functionalization of SWCNTs is an effective method to enhance this bonding. However, covalent bonds introduced by a functional group may alter the pristine structure of the SWCNT and affect its mechanical properties. Thus it is important to delineate effects of covalent functionalization on elastic properties of a SWCNT. We study here effects of covalent functionalization on Young's modulus, Poisson's ratio and shear modulus of a SWCNT in the graphitic plane. We consider hydrogen (–H), hydroxyl (–OH), carboxyl (–COOH), and amine ($–NH_2$) as model functional groups in this work. We use molecular mechanics (MM) simulations with the MM3 potential and the software TINKER to analyze simple tension and torsional deformations of pristine and functionalized SWCNTs. As is commonly assumed, we hypothesize that the response of a SWCNT to these deformations is the same as that of an energetically and geometrically equivalent continuum cylinder of wall thickness 3.4 Å. From curves of the strain energy density of deformation versus the axial strain and the shear strain for each functionalization group, values of Young's modulus and the shear modulus, respectively, are deduced. From results of the tension tests on a pristine and a SWCNT fully functionalized with hydrogen (–H), Poisson's ratio is computed. It is found that for each functional group studied and 20% functionalization, Young's modulus and the shear modulus decrease by about 34% and 43%, respectively, and Poisson's ratio of the functionalized SWCNT is more than that of the pristine SWCNT. These results should help in determining mechanical properties of SWCNT reinforced nanocomposites by using a micromechanics approach.

1. Introduction

Researchers have employed experimental and analytical techniques, density functional theory (DFT), molecular dynamics (MD) and molecular mechanics (MM) simulations to predict mechanical properties of carbon nanotubes (CNTs). Assuming that the wall thickness of a single-wall CNT (SWCNT) can be approximated as 0.34 nm, Treacy et al. [1], Wong et al. [2], and Krishnan et al. [3] experimentally determined that Young's modulus of a CNT is in terapascal (TPa) range. Xing et al. [4] employed MD simulations to predict Young's modulus of a SWCNT. Li and Chou [5] computed elastic properties of CNTs using combined structural mechanics and MM approach. Chang and Gao [6] investigated size dependent elastic properties of SWCNTs through MM simulations. Sears and Batra [7] determined the wall thickness, Young's modulus, and Poisson's ratio of CNTs using MM simulation with the MM3 potential and the software TINKER. They assumed that the responses of a SWCNT in simple tension and pure torsional deformations are energetically equivalent to those of a thin cylinder made of an isotropic and homogeneous material and of length, mean radius and thickness equal to those of the SWCNT. They found the wall thickness and Young's modulus of a SWCNT to be 0.046 nm and 7.26 TPa, respectively. Shen and Li [8] used MM potential and energy equivalent principle to determine values of five elastic constants of a CNT assuming the CNT as a transversely isotropic material with the centroidal axis of the tube as the axis of transverse isotropy. Batra and Sears [9] proposed that the axis of transverse isotropy of a CNT is a radial line rather than the centroidal axis. By studying with MM simulations radial expansion of a SWCNT, they showed that Young's modulus in the radial direction is about 1/4th of that in the axial direction. Gupta and Batra [10,11] predicted the material moduli of a SWCNT and the wall thickness of the equivalent continuum cylinder by matching frequencies of bending, axial and torsional vibrations as well as that of radial breathing modes of a free-free SWCNT with those of the equivalent continuous cylinder. As pointed out, amongst others, by Gupta and Batra [10,11], different techniques give varying values for the wall thickness of a SWCNT. Wu et al. [12] developed an atomistic based

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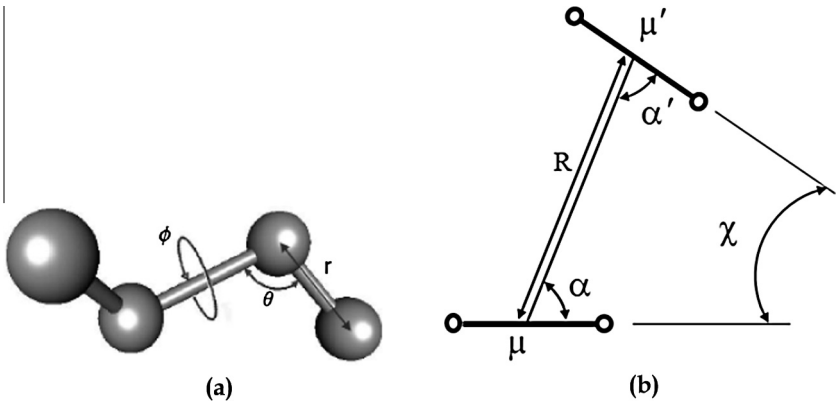

Fig. 1. Definitions of some variables in the MM3 potential. (a) Parameters r, θ and ϕ [7] and (b) parameters involved in dipole–dipole interaction [45].

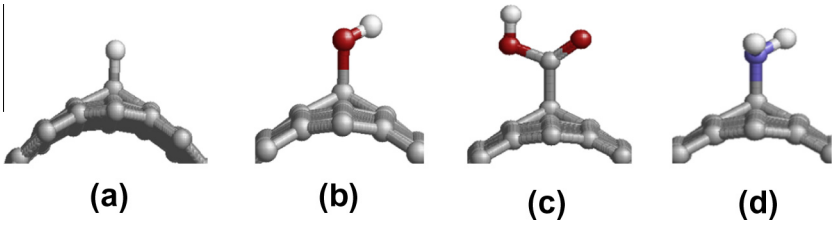

Fig. 2. Schematics of a carbon atom of the CNT attached with (a) hydrogen (–H), (b) hydroxyl (–OH), (c) carboxyl (–COOH), and (d) amine ($-NH_2$) groups.

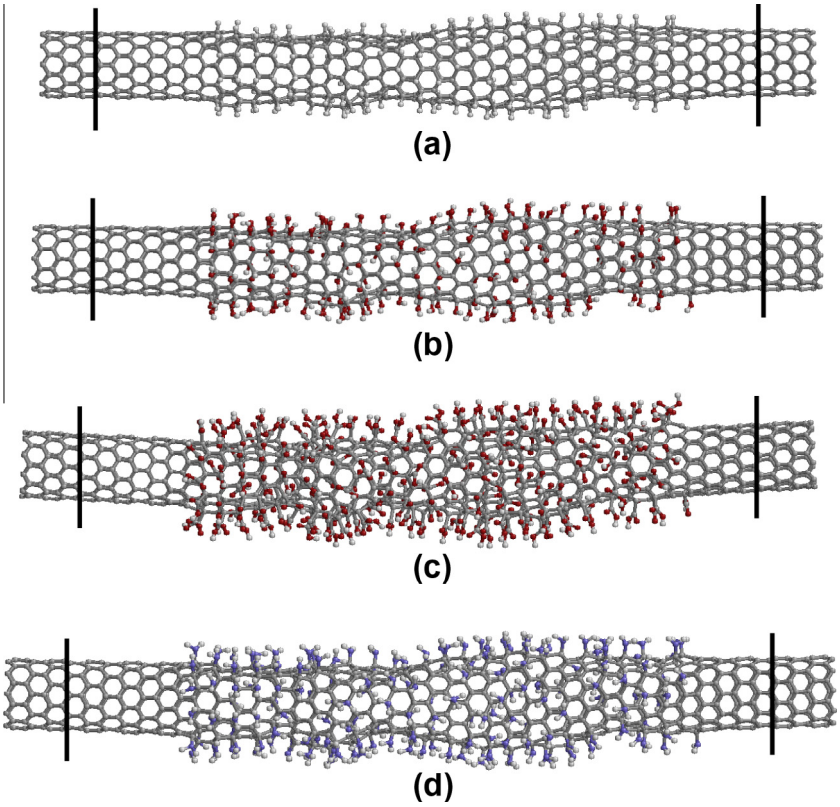

Fig. 3. Schematics of a (10, 0) SWCNT having 20% of randomly selected carbon atoms functionalized with (a) hydrogen (–H), (b) hydroxyl (–OH), (c) carboxyl (–COOH), and (d) amine ($-NH_2$) groups (Black vertical lines denote rings of carbon atoms where boundary conditions are specified).

finite deformation shell theory for a SWCNT and found its stiffness in tension, bending, and torsion.

The SWCNTs due to their cylindrical shape, large length to diameter ratio, and high specific properties are potential candi-