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Elastic and structural properties and buckling behavior of single-walled carbon nanotubes under chemical adsorption of atomic oxygen and hydroxyl

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ABSTRACT

Atomic decoration of carbon nanotubes (CNTs) is an effective way to alter the key properties of pristine CNTs. Elastic properties and axial buckling behavior of atomic oxygen and hydroxyl chemisorbed single-walled CNTs are explored employing molecular dynamics (MD) simulations. Our results demonstrate that the structure of chemisorbed CNTs changes compared to pristine CNT which considerably depends on the distribution pattern of chemisorbed oxygen and -hydroxyl. The results also demonstrate that chemisorption of atomic oxygen and -hydroxyl reduces Young's modulus and critical strain while increases the critical force of CNTs. Buckling mode shape of chemisorbed CNTs depends on the distribution pattern.

1. Introduction

Carbon nanotubes (CNTs) have been the subject of many interests in recent years due to their unique sp^2 hybridized atomic structures resulting in outstanding physiochemical properties like large specific surface area, high strength and thermal conductivity as well as extraordinary electronic properties. The specific structure of CNTs together with their exceptional properties makes them so promising for various industrial applications [1,2]. After many intense investigations on the intrinsic properties of pure CNTs, numerous researchers concentrated on developing the effective ways to control the properties of CNTs to apply them in certain applications and nanodevices. Functionalization is found to be a practical and efficient way to tailor the properties of nanostructures in order to use them in the wide range of applications in biotechnology and drug delivery nanodevices [3–12]. Functionalization can be performed through different methods such as doping or introducing any defects on CNTs, exohedral and endohedral polymer functionalization [13–17] and atomic-decoration [18–27]. It was observed that the intrinsic properties of host structures considerably change via introducing foreign atoms into CNTs, e.g. atomic decoration. Change in the sp^2 structure and also surface polarity in the case of chemisorption is mainly responsible for considerable alterations of intrinsic physiochemical properties. Among several possible decorations of CNTs, chemisorption of oxygen, known as oxygenation, is of great importance for its purification and reshaping capabilities of intrinsic CNTs. For some potential applications of carbon nanostructures, they must be highly purified. Oxidation process provides exceedingly purified CNTs and also increases the chemical reactivity of such graphitic surfaces [28,29]. Oxygen-containing groups, like hydroxyl, enhance the solubility of CNTs, especially in polar media. Besides, oxygen-containing group functionalization is a very crucial step for the enhancement of interfacial adhesion in nanocomposites [30]. Moreover, oxygenation alters the electronic, transport and emission properties of CNTs and hence is responsible for the construction of gas sensors built from CNTs [31]. Also, it is considered as the easiest way to covalent functionalization of CNTs with chemical groups like carboxylic acids. These functionalized groups can be used as base locations for further functionalization by other molecules [32]. In this regard, many experimental oxidation processes like wet chemical methods [32,15,33–36,28,37], photo oxidation [38,39], oxygen plasma [40], gas phase treatment [41] and theoretical investigations [42–48] have been carried out in recent years to study the possibilities of chemisorption of oxygen atoms and molecules on CNTs and their effects on structural and electronic properties.

Among the intrinsic properties of these nanostructures, mechanical properties are of the most determinant properties of such nanostructures in a proper design of new nanodevices using these modified nanostructures. Hence, in this investigation, the elastic properties (Young's modulus) and buckling behavior (critical force and strain, buckling mode shape) of chemisorbed CNTs

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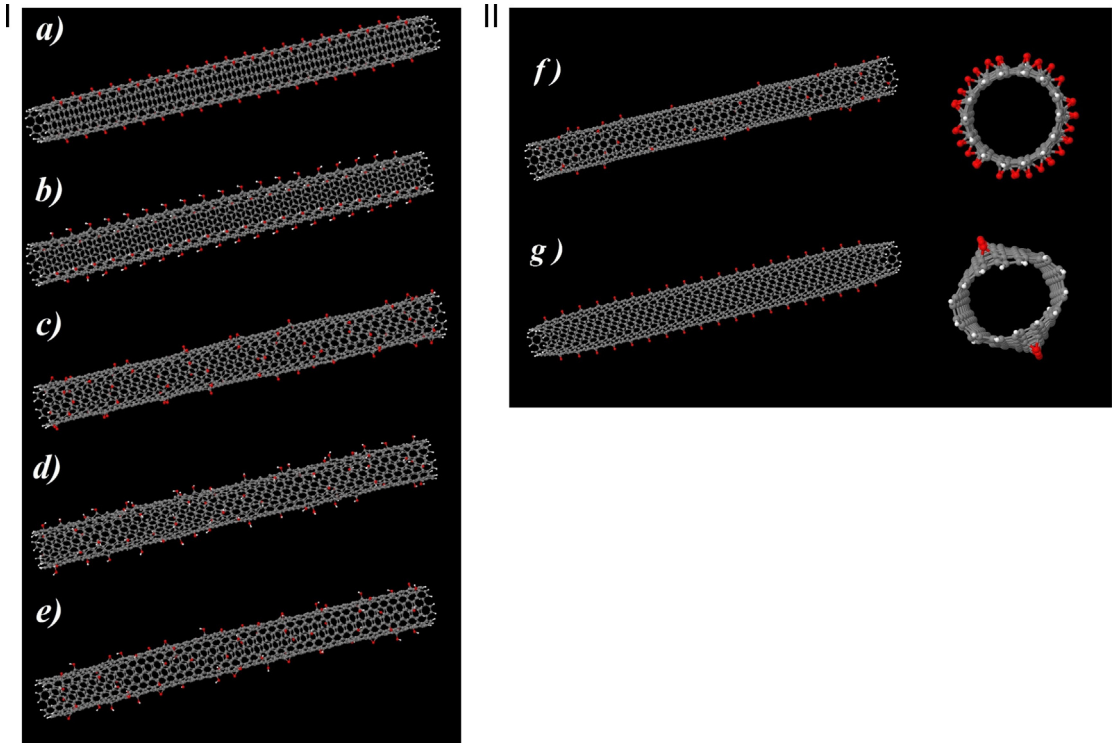

Figure 1. Schematic representation of I. (a) MO, (b) MOH, (c) RO, (d) ROH and (e) RO–ROH models, II. (f) random pattern and (g) regular pattern with 2% of oxygen.

by atomic oxygen and hydroxyl are explored utilizing molecular dynamics (MD) simulations which are not considered so far.

2. Methodology

In this investigation, Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) [49] is employed to perform classical molecular dynamics (MD) simulations. In this regard, AMBER force field [50] is chosen to calculate the energetics of nanostructure in the canonical ensemble (NVT) at the room temperature [51]. In order to guarantee the stability and reduction of temperature fluctuation of simulation system, Nose–Hoover thermostat algorithm is implemented within the Velocity-Verlet integrator algorithm and time step of 1 fs is selected [52–54]. Conjugate gradient algorithm with an energy convergence norm is also applied to minimize energy of simulation system in order to reach sufficient minimum relative energies. In all simulations, axial load is applied by imposing a displacement of 0.01 Å in a desired direction for tension and compression to the boundaries of CNTs and then the structure is allowed to relax for 5 ps. It should be noted that in these explorations, the CNTs are taken to be long enough so that the effect of boundary conditions and chirality of CNTs on the computed values can be neglected [55,56]. After relaxation, the energy of functionalized CNT in each step of loading is computed and the desired mechanical properties and buckling behavior are determined and also the buckling modes are illustrated.

3. Results and discussion

In this study, two types of possible oxygen atom and hydroxyl group chemisorbed on a (7,7) CNT with length of 110 Å, with different patterns and weight percentages are considered which are denoted by MO, MOH, RO–ROH, RO and ROH. The introduced abbreviations are explained as follows:

i. MO: regular pattern distribution of oxygen atoms on CNTs.
ii. MOH: regular pattern distribution of O—H (-hydroxyl) components on CNTs.
iii. RO–ROH: random pattern distribution of combination of oxygen atoms and O—H (-hydroxyl) components on CNTs.
iv. RO: random pattern distribution of oxygen atoms on CNTs.
v. ROH: random pattern distribution of O—H (-hydroxyl) component on CNTs.

The schematic of all models and difference between the regular and random patterns are presented in Figure 1. As revealed in this figure, regular pattern indicates that oxygen atoms are distributed in a row along the length of CNT uniformly and oxygen or hydroxyl concentration along the CNT is constant. Contrary to regular distribution patterns, in random distributions, there is no rule for the adsorption sites of oxygen and hydroxyl along the CNT; and components concentration along the CNT is not constant. To make a closer look to covalent bonding of models, Figure 2 is revealed. As it is observed from the minimization results of molecular dynamics simulations, single oxygen atoms can covalently bonded with two nearest carbon adjacent (Figure 2Ia) In the case of not being adjacent, minimization process reveals the destruction of hexagonal structure of functionalized CNT (Figure 2Ib). Also, O—H (-hydroxyl) component form covalent bond with a carbon atom on hexagonal structure of CNTs (Figure 2Ic). As presented in Figure 2II, initial relaxation of chemisorbed structures shows change in the structure of regular pattern distribution models. From this figure, it is observed that in MO models, circular cross section of CNTs changes to oval shape or noncircular soft corner shapes (Figure 2IIa) and an initial curvature is formed along the CNTs axis by increasing the weight percentage. Considering O—H (-hydroxyl) chemisorption, it is found that the cross-section changes to polygons with sharp corners (Figure 2IIb). In other configurations (random distributions), the circular shape of chemisorbed CNTs cross section is approximately preserved whereas the diameter increases slightly to its equilibrium value which is small enough and can be neglected.