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Elastic properties and buckling behavior of single-walled carbon nanotubes functionalized with diethyltoluenediamines using molecular dynamics simulations

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ABSTRACT

Carbon nanotube (CNT) modification processes are of great importance for good dispersion of CNTs and load transfer issues in nanocomposites. Among these processes, polymer covalent functionalization is found to be an effective way to alter the mechanical properties and behavior of pristine CNTs. Therefore, the mechanical properties and buckling behavior of diethyltoluenediamines (DETDA) functionalized CNTs are investigated employing molecular dynamics (MD) simulations. The results demonstrate that as the polymer weight percentage increases, Young's modulus and critical buckling load increase almost linearly for both regular and random polymer distributions, whereas critical strain decreases with different trends depending on the type of polymer distribution. Finally, the buckling mode shapes of the presented models are illustrated and it was revealed that there are some differences between the mode shapes of functionalized CNTs and those of pristine CNTs.

1. Introduction

Since the discovery of carbon nanotubes (CNTs) [1], their unique mechanical, electrical and structural properties have attracted much interest of researchers around the world. During the past

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two decades, it has been found that apart from the outstanding intrinsic properties of individual CNTs like extraordinary mechanical, optical and electrical properties, they demonstrate high potential applications in nanoelectronics, nanosensors, nanocomposites, energy storage systems and so on [2,3]. It was observed that CNTs can be used as a superlative reinforcer, together with polymers in a nanocomposite structure [4–6]. Practically, because of agglomeration tendency of CNTs to form bundles and also strong interaction between walls of tubes which result in limitation of their solubility and dispersion in a polymer matrix [3,7], CNTs applications in nanocomposites were restricted to a significant extent [8,9]. To overcome this, a great has been made to break these bundles in order to good dispersion and also improvement of load transfer in the desired matrices. In this regard, numerous investigations have been carried out for CNT modification in recent years [2,10–13]. Functionalization of CNTs is found to be an effective way of modification processes which in general is divided in two main categories: noncovalent and covalent functionalizations [2,9,14–17]. Generally, noncovalent functionalization is on the basis of different interactions like van der Waals (vdW) and electrostatic forces, hydrogen bonds and π stacking interactions [18–21] and includes surfactants [22], biomacromolecules [23] and wrapping with polymers [24,25]. This kind of functionalization takes the advantage of preserving the graphitic sp^2 structure compared to covalent functionalization. Besides, duo to π-orbitals of carbon atoms, CNTs are found to be reactive enough to form covalent bonds with other atoms [26]. By introducing the functional groups [27,28] to the CNTs, covalent functionalization can be formed based on two direct (covalent sidewall functionalization) and indirect (defect functionalization) methods [2,29–31]. Apparently, covalent functionalization destroys the perfect structures of CNTs resulting in significant changes in the mechanical, electrical and physical properties of CNTs as expected.

Covalent functionalization of polymer molecules, known as polymer grafting, possesses an important role in enhancement of polymer/CNT nanocomposites. To the best of authors' knowledge, investigation on the mechanical properties and buckling behavior of an individual functionalized CNT has not been studied in the literature up to now. Hence, in this paper the elastic properties and buckling behavior such as critical strength and strain of diethyltoluenediamines (DETDA) functionalized single walled carbon nanotube (SWCNT) which is successfully produced recently through diazonium-based addition quite [32], are investigated. Additionally, the effect of weight percentage of DETDA polymer on the aforementioned properties is studied in both random and regular patterns of covalent functionalization.

2. Methodology

In order to perform classical molecular dynamics simulations in this study, Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) [33] is employed. In all simulations, canonical ensemble (NVT) is chosen employing Amber force field [34] in order to calculate the energetics of corresponding nanostructure in the room temperature. Moreover, Nose–Hoover thermostat algorithm is implemented within the velocity-Verlet integrator algorithm and time step of 1 fs is chosen to guarantee the stability and reduction of temperature fluctuation of simulation system [35–37]. Also, to minimize energy of simulation system and in order to reach sufficient minimum relative energies, conjugate gradient algorithm with an energy convergence norm is applied. To simulate axial load, a displacement of 0.01 Å in desired direction for tension and compression is applied to the boundaries of functionalized CNT 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. 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 mode shapes are illustrated.

3. Results and discussion

In order to demonstrate the structure of functionalized CNTs, Fig. 1 is presented. This figure illustrates DETDA polymer structure, a pristine (7,7) CNT with length of 110 Å and schematics of