



Computational study of the effect of carbon vacancy defects on the Young's modulus of (6, 6) single wall carbon nanotube

Elvis G. Fefey, Ram Mohan*, Ajit Kelkar

Computational Science and Engineering, North Carolina A&T State University, Greensboro, NC 27411, United States

ARTICLE INFO

Article history:

Received 20 July 2010

Received in revised form 17 January 2011

Accepted 21 February 2011

Keywords:

SWCNT

Molecular dynamics

Young's modulus

Vacancy defects

ABSTRACT

Most molecular dynamics (MD) simulations for single wall carbon nanotubes (SWCNT) are based on a perfect molecular material structure. The presence of vacancy defects in SWCNTs could lead to deviations from this perfect structure thus affecting the predicted properties. The present paper investigates the effect of carbon vacancy defects in the molecular structure of SWCNT on the Young's modulus of the SWCNT using MD simulations performed via Accelrys and Materials Studio. The effect of the position of the defects in the nanotube ring and the effect of the number of defects on the Young's modulus are studied. The studies indicate that for an enclosed defect with the same shape in a SWCNT structure, its position did not cause any change in the Young's modulus. However, as the number of defects increased, the predicted Young's modulus was found to decrease. For a 10 ring (6, 6) SWCNT, six vacancy defects (corresponding to a defect percentage of 2.5%) reduced the Young's modulus by 13.7%.

© 2011 Elsevier B.V. All rights reserved.

1. Introduction

Since their discovery by Iijima in 1991 [1], single wall carbon nanotubes (SWCNTs) have gained significant attention because of their superior chemical, mechanical and thermo-physical properties [2]. Polymer nanocomposites formed with dispersion of SWCNT as reinforcement in a polymer matrix have been reported to result in significant improvement in mechanical and electrical properties compared to the original polymer matrix [3,4]. The higher mechanical properties and low specific weight make SWCNT a viable reinforcement in high performance composites [5]. The mechanical properties of SWCNTs and that of polymer nanocomposites containing SWCNTs have been studied through theoretical, experimental and computational analysis [6–9]. Results reported in the recent studies have indicated that mechanical properties obtained from experiments tend to be lower than those obtained from the computational analysis [9]. Several reasons have been assigned for this disparity including the fact that the experimental macroscopic coupons have SWCNTs dispersed in various orientations, while the computational models usually have the SWCNTs uni-directionally aligned. Another cause for this disparity is the fact that experimental processes could introduce defects into the SWCNTs, while computational

models are based on a perfect SWCNT molecular material structure.

Carbon vacancy defects in the molecular structure have been known to cause changes in the behavior and properties of CNTs [10–14]. Mielke et al. [10,11] explored the role that missing atoms have in the fracture of defective CNTs through quantum mechanical calculations using density functional theory, semi-empirical methods, and molecular mechanics. One and two atom vacancy defects in the CNTs were reported to reduce failure stresses by as much as approximately 26% with markedly reduced failure strains. It was also demonstrated that large holes, such as those that might be introduced through oxidative purification processes, greatly reduced the strength of the carbon nanotubes. In the work of Park et al. [13], carbon nanotubes with vacancy defects were found to be most suitable as platinum carrier electrodes in fuel cells. This result was based on the finding that the binding energies at defect sites were greater; this resulted in enhanced adsorption on defective SWCNTs. The binding energy on defective SWCNTs was always larger than that on pure SWCNTs, with the binding energy at vacancy sites about twice that of any other configuration.

As noted above, defects in CNTs have an impact on their mechanical properties and understanding their influence on the Young's modulus is the focus of the present paper. The objective of the present work is to investigate the influence of vacancy defects in SWCNT on their mechanical properties, in particular Young's modulus. This is achieved through quantitative evaluation of the mechanical properties via computational molecular dynamics (MD) modeling of (6, 6) single wall carbon nanotube (SWCNT) with and without vacancy defects.

* Corresponding author at: 319 Fort IRC Building, 1601 E Market Street, North Carolina A&T State University, Greensboro, NC 27411, United States.
Tel.: +1 336 334 7437; fax: +1 336 256 1247.

E-mail addresses: rvmohan@ncat.edu, rmohanncat@gmail.com (R. Mohan).

2. Computational molecular dynamics modeling and atomistic model configurations

Molecular dynamics (MD) modeling provides in detail the dynamic individual particle motions and structure developments as a function of time [14] and therefore serves as a great tool to study the properties of a material system. Several prior work of CNT dynamics are noted in the literature, with large numbers of computational studies based on molecular dynamics simulations. Prylutsky et al. studied the mechanical, vibrational, and electronic properties of (5,5) and (10,0) nanotubes with molecular dynamics [15]. Yao et al., studied mechanical properties of SWCNT with a diameter of 1.2 nm and length 4.7 nm via MD simulations [16]. Interfacial resistance between carbon nanotubes was studied using MD simulations by Zhong and Lukes [17]. Xia and Liang studied the MD and multi-scale modeling of carbon nanotube adhesion for dry adhesives [18]. In the MD simulations, all degrees of freedom due to the electrons are ignored, as well as quantum effects; are best suited for large systems and are fast and computationally cheaper compared to the other first principle methods. The method also makes it feasible to model and analyze larger scale molecular models involving cross-linked polymer systems and composite systems with CNT. The electron freedoms are incorporated and accounted through empirical potentials. Other *ab initio* methods such as density functional theory (DFT) are time consuming and consider more details about the electrons and ions; can give more interactions and corrections about electron–electron, electron–ion, and ion–ion. However, they are limited to static states of small systems, slow and expensive [19]. The present work employs molecular dynamics modeling that has been used in several other studies on computational modeling with carbon nanotubes reported in the literature [6–9,15–19].

2.1. Creation and simulation of pure SWCNT atomistic model configuration

All molecular models were created in Materials Studio (version 4.4) and molecular modeling analysis simulations were conducted using Discover module by Accelrys Inc. A unit cell of the (6, 6) SWCNT was created in Materials Studio, followed by the generation of a super cell built with 10 SWCNT unit cells. The resulting carbon nanotube had a length of 23.4 Å, diameter of 8.14 Å, and a bond length of 1.42 Å. Fig. 1 shows the unit cell and super cell generated and modeled with Materials Studio. All angles of the cell were made equal to 90° to ensure a rectangular box.

2.1.1. Potential energy characterization

The potential energy of the molecular models is characterized by the COMPASS force field [20] with the non-bond energies characterized by the van der Waals and Coulomb's interactions. COMPASS (condensed-phase optimized molecular potentials for atomistic simulation studies) is a member of consistent family of force fields (CFF91, PCFF, CFF and COMPASS). This force field is a quantum mechanical force field which facilitates accurate prediction of structural, conformational, vibrational, and thermophysical properties for a broad range of molecules in isolation and in condensed phases. In the present MD simulations with Accelrys, SWCNT structure was parameterized using force field CFF91. The total energy functional form for the general CFF91 force field consists of terms for bonds (b), angles (θ), torsion angle (ϕ), and out-of-plane angle (χ), as well as cross-terms, and two non-bond interactions that include the van der Waals (vdW) and electrostatic interaction. The general functional form for CFF91 force field is

given by [20]:

$$E_{\text{Total}} = E_b + E_\theta + E_\phi + E_\chi + E_{b,b'} + E_{b,\theta} + E_{b,\phi} + E_{\theta,\phi} + E_{\theta,\theta'} + E_{\theta,\theta',\phi} + E_q + E_{\text{vdW}} \quad (1)$$

The various terms for the CFF91 force field are given by [20]

$$\begin{aligned} E_b &= \sum_b [k_2(b - b_0)^2 + k_3(b - b_0)^3 + k_4(b - b_0)^4] \\ E_\theta &= \sum_\theta [k_2(\theta - \theta_0)^2 + k_3(\theta - \theta_0)^3 + k_4(\theta - \theta_0)^4] \\ E_\phi &= \sum_\phi [k_1(1 - \cos \phi) + k_2(1 - \cos 2\phi) + k_3(1 - \cos 3\phi)] \\ E_\chi &= \sum_\chi k_2\chi^2 \\ E_{b,b'} &= \sum_{b,b'} k(b - b_0)(b' - b'_0) \\ E_{b,\theta} &= \sum_{b,\theta} k(b - b_0)(\theta - \theta_0) \\ E_{b,\phi} &= \sum_{b,\phi} (b - b_0)(k_1 \cos \phi + k_2 \cos 2\phi + k_3 \cos 3\phi) \\ E_{\theta,\phi} &= \sum_{\theta,\phi} (\theta - \theta_0)(k_1 \cos \phi + k_2 \cos 2\phi + k_3 \cos 3\phi) \\ E_{\theta,\theta'} &= \sum_{\theta,\theta'} k(\theta' - \theta'_0)(\theta - \theta_0) \\ E_{\theta,\theta',\phi} &= \sum_{\theta,\theta',\phi} k(\theta - \theta_0)(\theta' - \theta'_0) \cos \phi \\ E_q &= \sum_{i,j} \frac{q_i q_j}{r_{ij}} \end{aligned} \quad (2)$$

$$E_{\text{vdW}} = \sum_{i,j} \varepsilon_{ij} \left[2 \left(\frac{r_{ij}^0}{r_{ij}} \right)^9 - 3 \left(\frac{r_{ij}^0}{r_{ij}} \right)^6 \right] \text{ where}$$

$$r_{ij}^0 = \left(\frac{(r_i^0)^6 + (r_j^0)^6}{2} \right)^{1/6}$$

$$\varepsilon_{ij} = 2\sqrt{\varepsilon_i \varepsilon_j} \left(\frac{(r_i^0)^3 (r_j^0)^3}{(r_i^0)^6 (r_j^0)^6} \right)$$

The corresponding CFF91 force field parameters for the C–C bonds as obtained from Accelrys for the carbon nanotube analysis is listed in Table 1. All the parameter values as defined by CFF91 within Accelrys analysis software are directly used. Table 1 lists values for the C–C bonds as available and obtained from the CFF91 force field parameter file named “cff91.frc” in Accelrys analysis software.

2.1.2. Energy minimization

Based on the total potential energy of the molecular model defined through the force field as discussed earlier, the energy of the super cell SWCNT molecular structure was minimized to obtain the most stable energy configuration. This was achieved through minimization of the potential energy function using a cascade of the steepest descent minimization method and the Fletcher–Reeves

Download English Version:

<https://daneshyari.com/en/article/1529913>

Download Persian Version:

<https://daneshyari.com/article/1529913>

[Daneshyari.com](https://daneshyari.com)