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Buckling of defective carbon nanotube

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Abstract

Carbon nanotube (CNT) has attracted enormous attention from researchers since its discovery in 1991. Due to their remarkable mechanical properties, carbon nanotubes have been employed in many diverse areas of applications including biological probes, atomic force microscopy and also in nanocomposites. However, similar to any of the many man-made construction materials used today such as steel and concrete, carbon nanotubes (CNTs) are also susceptible to various kinds of defects.

Understanding the effect of defects on the mechanical properties of CNTs is essential in the design of nanotube-based structures. It has been found in various past studies that these defects can affect considerably the tensile strength and fracture of CNTs. Comprehensive studies on the effect of defects on the buckling and vibration of nanotubes is however lacking in the literature. In this paper, the effect of atomic vacancy defect on the axial buckling of single-walled carbon nanotubes (SWCNTs) is investigated using molecular dynamics simulations. COMPASS force field in Material Studio commercial software is employed for the molecular dynamics simulations.

Results obtained in the present study revealed that even a single missing atom can cause a significant reduction in the critical buckling strain and load of SWCNTs. As the number of missing atoms increases, the percentage reduction of buckling strain and load due to each missing atom reduces. Moreover, due to the higher flexibility resulted from more missing atoms, significant strain energy drop cannot be observed at the buckle. However, drop of load can still be observed at the buckle even for the SWCNTs with more missing atoms. Moreover, as the number of missing atoms increases non-linear portion can be seen in the load displacement curve before buckle.

Keywords: defective nanotubes, buckling, molecular dynamics simulations

1 Introduction

Carbon nanotube (CNT) is a nanomaterial that attracts enormous attention of researchers in the last two decades. It is now well known that carbon nanotubes posses superior mechanical, electrical and thermal properties. These properties have spurred considerable interests among researchers and as a result, many experimental and theoretical studies have been performed so far to explore these remarkable material properties. However, as in any other man made products, carbon nanotubes are also known to be susceptible to defects. Studies have revealed the existence of various kinds of defects such as missing atoms (vacancy defects), presence of carbon rings other than usual hexagonal rings (Stone-Wales defects) or presence of sp3 bonds instead of usual sp2 bonds (rehybridization defects). Interestingly, in spite of the degradation in strength and stiffness caused by these defects,

defects are found to be favorable in some situations. For example, vacancy or rehybridization defects are found to increase the bonding between nanotube and matrix in the case of nanotube based composites and load transferring ability in the case of multi-walled carbon nanotubes and nanotube bundles. Defects can occur in nanotubes during production or purification. Some defects are produced in an excessive temperature environment or under high stresses. Also, defects can be deliberately introduced by chemical treatment or irradiation.

Many studies have been conducted to explore the effect of defects on the tensile properties and fracture of carbon nanotubes. Belytschko et al (2002) used molecular mechanics based on Morse and Brenner potentials to study the fracture of CNT and found that even a single missing atom can reduce its strength by about 25%. Similar observations have been made by Meo and Rossi (2006) through molecular mechanics based finite element model and Xiao and Hou (2006) through molecular dynamics simulations (MDS). Moreover, Wang et al (2007) studied the fracture of achiral single-walled carbon nanotubes (SWCNT) with single atomic vacancy defect using molecular mechanics and a continuum shell model. Also, they studied the effect of defect location on fracture. Sammalkorpi et al (2004) studied the tensile strength and Young's modulus of SWCNTs with vacancy defects using MDS and derived analytical expressions for Young's modulus of defective CNT based on continuum theory. In their study, non-reconstructed defects, reconstructed defects and influence of different defect concentrations are investigated. Furthermore, they concluded that defects do not affect Young's modulus significantly but affect the tensile strength significantly. Zhang et al (2005) investigated the effects of one and two-atomic vacancy defects and slits and holes on fracture of single-walled CNT, double-walled CNT (DWCNT) and triple-walled CNT (TWCNT) using atomistic simulations and multi-scale methods.

However, only few works on the effect of defects on buckling of CNTs can be found in the literature. Hirai et al (2003) has studied the influence of two types of pin-hole defects on the tensile strength, buckling strength and resonant frequency of SWCNTs with different chiralities. Their study revealed that there is a significant reduction in the above mentioned properties caused by the presence of defects. Hao et al (2008) studied the effect of single atom vacancy defect on the buckling of SWCNT and DWCNT using MDS based on Morse potential. They have observed significant effect on buckling load and buckling strain especially in small tubes. They further concluded that the relative positions of defects in the inner and outer walls play an important role in the buckling of DWCNTs. Wang et al (2008a) have also studied the effect of single atomic vacancy defect on the buckling of (8, 0) SWCNT using MDS and continuum beam model. However, their results do not show considerable effect of defect on buckling strain of CNTs.

The aim of this paper is to explore the effect of vacancy defects arising from missing carbon atoms on the buckling properties of CNTs using MDS based on COMPASS force field. The effect of increasing number of missing atoms on the critical buckling strain and critical buckling load of SWCNT is the primary focus of this paper.

2 Atomic simulation model

In the present study, COMPASS (condensed-phase optimized molecular potentials for atomistic simulation studies) force field in Material Studio 4.4 is used for the simulation. COMPASS force field has been proven as a better force field for analyzing mechanical behavior of CNTs and has been used by many researchers (Cao and Chen, 2006a, 2006b; Chen and Cao, 2006; Wang et al, 2007, 2008a, 2008b, Kulathunga et al, 2009). This force field accounts for the cross-term interacting energy while the other widely used force field such as Tersoff-Brenner potential or Morse potential accounts only for valence energy (bond energy).

Molecular dynamics simulation in this study is done using a time step of 0.5fs and a compression rate of 1x10-3 nm/ps. Berendsen thermostat is used to maintain the environmental temperature. (7, 7)

SWCNTs with length 6.15nm are considered here. Defect is introduced approximately at the middle of the tube.

3 Results and discussion

Buckling of defective (7, 7) SWCNTs with 1, 2 and 3 missing atoms are studied here. The defect configurations are given in figure 1. Results were compared with pristine (7, 7) SWCNT.

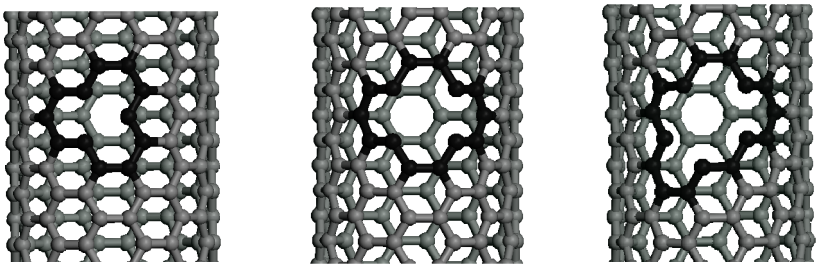

Figure 1: Defect configurations with 1, 2 and 3 missing atoms respectively.

The strain energy curves obtained from MDS are shown in figure 2.

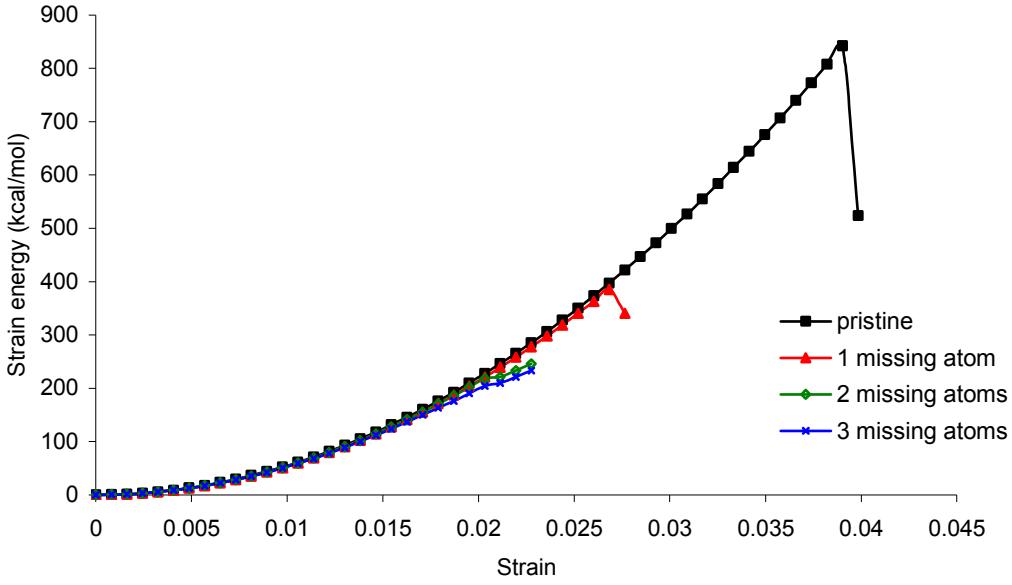

Figure 2: Strain energy curves for pristine and defective SWCNTs

Generally, a sudden drop of strain energy is found to occur at the point of buckle. Therefore, it can be seen from figure 2 that the critical buckling strain of pristine CNT is 0.04. This value is in reasonable agreement with the value (i.e. 0.05) obtained by Yokobson et al (1996) for the same SWCNT with approximately same length. It is evident from figure 2 that even the presence of single missing atom creates a significant decrease in buckling strain. As can be seen from the figure, the reduction of buckling strain due to one missing atom is 31%. This value is also in reasonable agreement with the value (i.e. 43.9%) obtained by Hao et al (2008) for the same SWCNT with approximately same length. For SWCNTs with two and three missing atoms, the strain energy drop at point of buckle is

not evident. In order to understand this discrepancy, detailed analysis of energy profile was conducted. It was understood from the results that at the point of buckle, both bond stretching energy and angle bending energy decreases while bond torsion energy and bond inversion energy increases. For pristine SWCNT and for defective SWCNT with one missing carbon atom, the increase in torsion and inversion energy is much lesser compared to the decrease in bond and angle energy and hence a net reduction of strain energy occurs. However, for SWCNTs with two and three missing atoms, the reduction in bond and angle is slightly lesser than the increment in torsion and inversion energy and hence a drop of strain energy cannot be seen from the figure. This is due to the higher freedom in motion achieved by carbon bonds near the defect as the number of missing atom increases.

Generally, the drop of force at the point of buckle is more evident than the drop of strain energy. Therefore, to determine accurately the buckling point of SWCNTs with two and three missing atoms, force displacement curves were also drawn and investigated. These curves are presented in figure 3.

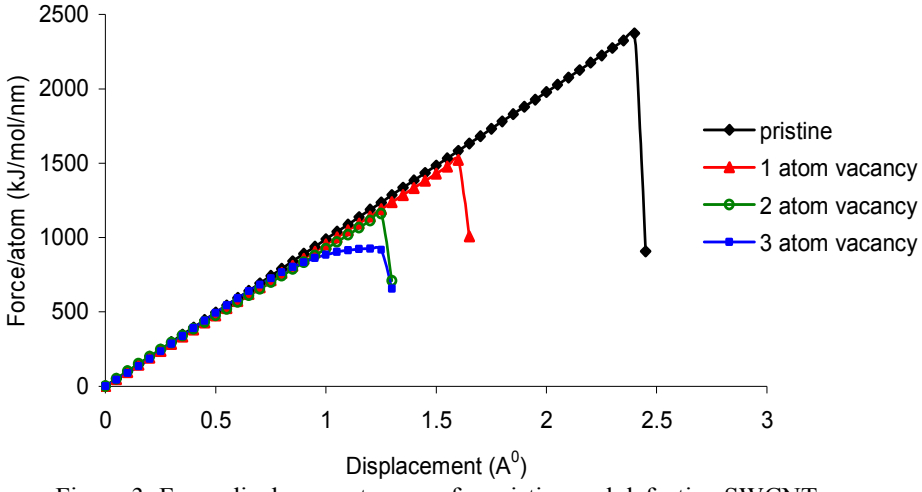

Figure 3: Force displacement curves for pristine and defective SWCNTs

It can be seen from figure 3 that SWCNT with two missing atoms do show a significant reduction of critical buckling strain compared to the tube with one missing atom. However, SWCNT with three missing atoms shows the same critical buckling strain as that with two missing atoms. Even though the critical buckling strains are the same, the critical buckling load of SWCNT with three missing atoms is lower than that of SWCNT with two missing atoms. Moreover, a nonlinear force displacement relationship can be observed for the SWCNT with three missing atoms before buckle. This is because the tube becomes more flexible as the result of more missing atoms.

4 Conclusion

Axially compressed buckling behaviour of (7, 7) SWCNT with vacancy defects resulting from 1, 2 and 3 missing atoms was studied in the present work. It is realized from the results that even a single missing atom can create a significant reduction in the critical buckling strain and buckling load of SWCNTs. However, as the number of missing atoms increases, the reduction of buckling strain and buckling load resulting from each increasing missing atom reduces. Moreover, nanotubes with more missing atoms seem to show a non-linear force displacement relationship before buckling due to the higher flexibility resulting from the defect.

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