Current Applied Physics 15 (2015) 1216–1221

Contents lists available at ScienceDirect

Current Applied Physics

journal homepage: www.elsevier.com/locate/cap

Simulation of mechanical properties of carbon nanotubes with superlattice structure

H. Xi [a], H.Y. Song [a, b, *], R. Zou [a]

[a] School of Science, Xi'an University of Posts and Telecommunications, Xi'an 710121, China
[b] College of Materials Science and Engineering, Xi'an Shiyou University, Xi'an 710065, China

ARTICLE INFO

Article history:
Received 22 May 2015
Received in revised form
23 June 2015
Accepted 5 July 2015
Available online 8 July 2015

Keywords:
Carbon nanotube
Mechanical property
Molecular dynamics simulation

ABSTRACT

The effect of radius and layer thickness on the mechanical properties of carbon nanotubes with 'zigzag-armchair-zigzag' superlattice structure (CNTSS) is investigated using molecular dynamics simulation method. The interactions between carbon atoms are modeled using the second-generation reactive empirical bond-order Brenner potential coupled with the Lennard-Jones potential. The results indicate that the Young's modulus of CNTSS shows a significant dependence on its radius and layer thickness. In contrast, the critical stress is insensitive to the layer thickness and radius of CNTSS. And the critical stress of CNTSS is close to that of its thicker carbon nanotubes segment. In addition, the damage modes of CNTSS depend on the connecting region due to the presence of 5–7 defects and the energy early concentrating in the junctions. The effects of the number of junctions on the mechanical properties of CNTSS are also discussed. The results indicate that the joints made in this way still have relatively high mechanical properties corresponding to that of the ideal single-walled carbon nanotube.

1. Introduction

Since the first report of carbon nanotube (CNT) by Iijima [1], the research on CNTs has attracted attention much due to the unusual mechanical, thermal, electronic properties [2–10]. Both theoretical and experimental studies indicated that CNTs are material with extreme Young's modulus and axial strength [11–13]. Although the CNT has excellent properties, it fails to satisfy the application requirements of nanoscale electronics circuits and devices. How to seamlessly connect two different CNTs together is quite urgent for us today. Two CNTs can be joined into an intramolecular junction (IMJ) by introducing one or multiple Stone-Wales (S–W) defects (pentagon and heptagon pair). Sharma et al. [14] investigated the mechanical behavior of pristine and defective single-walled CNTs under axial tensile using molecular dynamics (MD) simulation. Their results show that the defects reduce the strength and strain of CNTs, and vacancy defects are found to degrade CNTs to a greater extent than S–W defects. The S–W defects of IMJs are similar to the twin boundary of metal, which have smaller interfacial energy and affect the mechanical properties of the material slightly. The IMJs may exhibit different interesting characteristics due to the different chirality of the IMJ segments. Fu et al. [15] prepared the Y-junctions CNTs by direct pyrolysis of methane without adopting any catalyst using microwave CVD method. Yang et al. [16] investigated electronic properties by using a tight binding-based Green's function approach and found that the conductance of metal–metal IMJs is very sensitive to the connectivity of the matching tubes. The work of Yao et al. [17] demonstrated that a metal–semiconductor junction behaves like a rectifying diode with nonlinear transport characteristics. Hu et al. [18] studied the quantum conductance oscillations (QCOs) of the IMJs. The results indicated that the IMJs kept not only the high QCO frequencies in SWCNT, but also induced their sum frequencies. Zhou et al. [19] studied the thermal conductivity of (2n,0)-(n,n)-(2n,0) IMJs by using nonequilibrium MD approach. The results show that when the length of the middle tube is more than 3 nm, the thermal conductivity is only affected by the IMJs.

The atomic structural, electrical, optical and thermal properties of IMJs [15–24] have been extensively investigated and the IMJs offer a prospective future of CNT-based network in large-scale nanoelectronic devices. It is well known that the mechanical properties of IMJs are the basis for developing CNT-based nano-electro-mechanical system devices. However, the studies on the mechanical characterization of IMJs are still limited. Kinoshita et al.

* Corresponding author. School of Science, Xi'an University of Posts and Telecommunications, Xi'an 710121, China.
E-mail address: gsfshy@sohu.com (H.Y. Song).

http://dx.doi.org/10.1016/j.cap.2015.07.008
1567-1739/

[25] investigated the mechanical properties of CNT-IMJs by using first-principles density functional theory. The results show that the tensile strength and breaking strain of CNT-IMJs depend on the position of 5–7 defects, while these properties of CNT-IMJs are not significantly affected by the number of 5–7 defects. Qin et al. [26] studied the mechanical properties of CNT-IMJs by using MD simulations. They found that the rupture strain decreases and the Young's modulus increases with the decrease of the diameter ratio of the two constituent CNT segments. Kang et al. [27] investigated the buckling behavior of IMJs under axial compression by using MD simulation and finite element analysis. The results show that the critical compressive strain is sensitive to the strain rate under high-speed compression. However, the related study on the mechanical properties of the coaxial 'zigzag-armchair-zigzag' CNTSS is still very rare. Here, we investigate the effect of radius and layer thicknesses on the mechanical behavior of the coaxial 'zigzag-armchair-zigzag' CNTSS under tension loadings by using MD simulations. Some interesting results are obtained. The general conclusions derived from this work may provide a guideline for the preparation of large-size CNT.

2. Simulation model and MD method

The coaxial CNTSS ((2n,0)-(n–n)-(2n,0)) consisting of four (n,n) armchair and five (2n,0) zigzag CNTs is connected with alternating spaced pentagon and heptagon rings, as shown in Fig. 1. Here, the difference in the radii of the (n,n) and (2n,0) CNTs can be expressed as:

$$\Delta R = \sqrt{3}a_{c-c}n\left(2-\sqrt{3}\right)\Big/2\pi, \tag{1}$$

where a_{c-c} is the C–C bond length, is of 0.142 nm [28], n is integers called the CNT index. The radius of CNTSSs is average of its zig and arm CNTs segment, the CNTSSs radius is expressed by:

$$r = \frac{r_{zig} + r_{arm}}{2}, \tag{2}$$

A CNT-based junction is formed by connecting CNTs of one zigzag and one armchair through introduction of pentagon and heptagon rings into the connecting region, all those CNTSSs have open ends. In this work, we investigated the effect of radius and layer thicknesses on the mechanical behavior of the CNTSSs using MD simulations. The overall length of junction is defined as:

$$L = 4L_{thin} + 8L_{connecting} + 5L_{thick}, \tag{3}$$

where L_{thin}, $L_{connecing}$ and L_{thick} are the lengths of the thinner tube (armchair), the connecting region and the thicker tube (zigzag), respectively. Here, the length scale of CNTSS ranges from 11.23 to 30.07 nm according to the different layer thicknesses.

The selection of potential function is a key factor. In the simulations, the Brenner second-generation reactive empirical bond-order potential [29] is used for modeling the carbon–carbon bonded interaction. The nonbonded carbon–carbon interactions are described by a Lennard-Jones pair potential [30]. The expression for the total energy of the CNTSS system is written as:

$$E = \frac{1}{2}\sum_{j}\sum_{j\neq i}\left(E_{ij}^{\text{Tersoff-Brenner}} + E_{ij}^{LJ}\right), \tag{4}$$

here, the inter-atomic forces are modeled with the covalent bonding interactions is defined as

$$E_{ij}^{TB} = V_R(r_{ij}) - b_{ij}V_A(r_{ij}), \tag{5}$$

where r_{ij} is the distance between pairs of nearest-neighbor carbon atoms i and j, b_{ij} is a many-body empirical bond order term and depends on the bonding environment around atom i and j, the functions $V_R(r_{ij})$ and $V_A(r_{ij})$ are pair-additive interactions that represent all repulsion and attraction interactions. The aforementioned pair-additive are defined as

$$V_R(r_{ij}) = f_c(r_{ij})\left(1+\frac{Q}{r_{ij}}\right)A\exp^{-\alpha r_{ij}}, \tag{6}$$

$$V_A(r_{ij}) = f_c(r_{ij})\sum_{n=1}^{3}B_n\exp^{-\beta_n r_{ij}}, \tag{7}$$

where Q, B_n, α, β_n and A are constant parameters. In addition, the function $f_c(r_{ij})$ is a cut-off function, and is given by

$$f_c(r_{ij}) = \begin{cases} 1, & (r_{ij} < R_{ij}), \\ \frac{1}{2}\left[1+\cos\frac{\pi(r_{ij}-R_{ij})}{S_{ij}-R_{ij}}\right], & (R_{ij} < r_{ij} < S_{ij}), \\ 0, & (r_{ij} > S_{ij}), \end{cases} \tag{8}$$

In the Brenner potential, the cut-off function $f_c(r_{ij})$ in Eq. (8) introduces a dramatic increase in the interatomic force near the bond breaking length. Therefore, we use $R_1 = R_2$ in order to avoid overestimating the force required for bond breaking. In addition, the long range interactions between carbon atoms are calculated by L-J potential only if the covalent potential is zero. The L-J potential is expressed by:

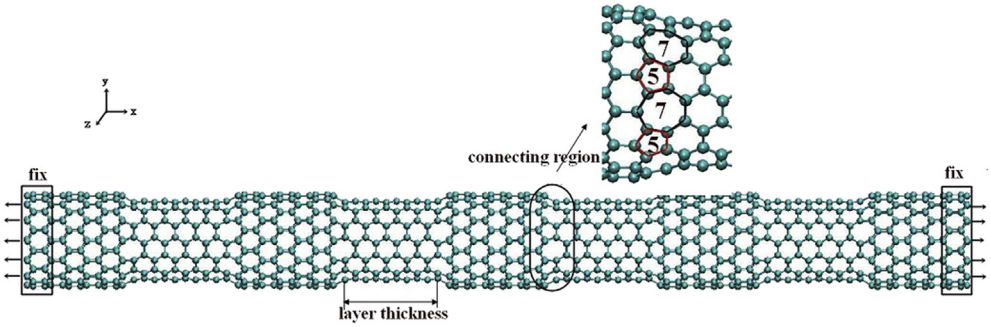

Fig. 1. Illustrations of the atomic structure.