Composite Structures 92 (2010) 1701–1705

Contents lists available at ScienceDirect

Composite Structures

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

Comparative MD simulation study on the mechanical properties of a zigzag single-walled carbon nanotube in the presence of Stone-Thrower-Wales defects

Keka Talukdar, A.K. Mitra *

Department of Physics, National Institute of Technology, Durgapur 713209, India

ARTICLE INFO

Article history:
Available online 23 December 2009

Keywords:
Stone-Thrower-Wales defects
Mechanical properties
CNT composite

ABSTRACT

Using molecular dynamics simulation, we investigate the influence of Stone-Thrower-Wales defects in the mechanical behavior of a zigzag (5, 0) single-walled carbon nanotube considering two different interatomic potential functions, the Tersoff–Brenner bond order potential and the Tight-Binding potential. The nanotube is subjected to axial stretch and the potential energy is computed for gradually increasing values of strain. From the energy–strain curve the mechanical characteristics like Young's modulus, tensile strength and ductility are computed using both the potentials, firstly with a perfect lattice and then by introducing an increasing number of Stone-Thrower-Wales defects. Significant reduction in the values of the mechanical properties is observed with changes in the plastic deformation pattern. Experimental data compares reasonably well with our calculated values of the mechanical constants. Such investigations will help designing carbon nanotube based composites.

© 2009 Elsevier Ltd. All rights reserved.

1. Introduction

Using carbon nanotubes (CNT) as reinforcing agents to design and fabricate strong composites with desirable mechanical properties needs thorough understanding of the mechanical behavior of such nanotubes. Topological defects such as Stone-Thrower-Wales (STW) [1] defects that are either inherently present in the CNTs or introduced into them in the manufacturing process; degrade their mechanical properties to a large extent. Such defect is produced by 90° rotation of a C–C bond and thus forming two pentagons and two heptagons (Fig. 1a and b).

Although many theoretical and experimental studies have been carried out to explore the mechanical behavior of carbon nanotubes, a wide variation in their results have been reported so far showing discordances of the theoretical values with the experimental ones. Theoretical studies [2–7] show a wide range of Young's modulus from 0.1 to 5.5 TPa while tensile strength varies from 5 to 150 GPa, depending on the different methods of calculation, different CNT chiralities or lengths and different potentials employed to define the C–C bond in the plane of the graphene sheets. Theoretically overestimated values of nanotube properties can be attributed to the presence of various defects in the CNT structures. The role of vacancy defects or holes on the mechanical properties of CNTs was studied in many theoretical investigations such as of Mielke et al. [8], Lee et al. [9], Xiao and Hou [10] and Wang et al. [11]. The contribution of different authors in this field is tabulated in Table 1.

As the exact knowledge of the stiffness or strength of the nanotubes is important for their use as the reinforcements in the next generation composites, and as the defects in general improve the adhesion of the CNTs to a polymer matrix [30], the defects are deliberately introduced into CNTs to achieve certain functionality. Moreover, defects may serve as a mediator to form a strong covalent bond for single-walled (SWCNT) or multi-walled (MWCNT) carbon nanotube bundles and thus improve their mechanical performances. Defects are easy to create, either chemically or by other processes they can be introduced in the CNT structure. Adding suitable number of STW defects, a CNT can be fully exploited for various applications. In this paper the dependence of the mechanical properties on the STW defects of a zigzag single-walled carbon nanotube (SWCNT) is studied with Tersoff–Brenner (TB1) potential and Tight-Binding potential (TB2) and the results are compared.

2. Method of calculation

This is a fact that no potential is developed so far that suits all scenarios. We have used the potential form developed by Brenner [31] for hydrocarbon, known as Tersoff–Brenner potential. Brenner's bond order potential function describes the bonding between the atoms of CNTs. It also describes the construction and destruction of bonding interaction between atoms. Though it lacks the inclusion of a long range molecular interaction, it enables us to simulate a wide range of deformations of a CNT under external

* Corresponding author. Tel.: +91 9434788002.
E-mail addresses: akmrecdgp@yahoo.com, profakm@nitdgp.ac.in (A.K. Mitra).

0263-8223/$ - see front matter © 2009 Elsevier Ltd. All rights reserved.
doi:10.1016/j.compstruct.2009.12.008

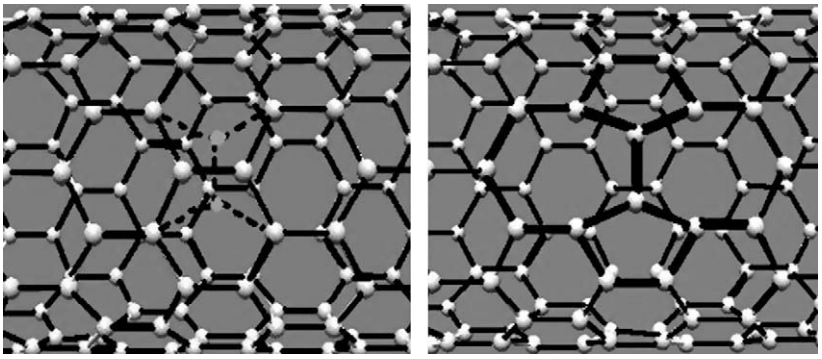

Fig. 1. (a) A defect free (5, 0) SWCNT (the dotted line shows the rotation of the bond by 90° (b) A (5, 0) SWCNT with a STW defect.

Table 1
Review of the work of some authors in the field of mechanical properties of SWCNTs.

Authors	Year	Method	Major contributions
1. Treacy et al. [12]	1996	TEM measurements (experimental)	Measured Young's modulus first as 1.81 TPa
2.Wong et al. [13]	1997	Experimental (AFM)	Measured *Y* value was 1.28 TPa
3. Nardelli et al. [14]	1997	By quantum and classical simulations	Noticed SW rotations beyond 5% strain which could produce plastic deformation in CNTs
4. Zhang et al. [15]	1998	Tight binding MD simulation	Dependence of plastic deformation on wrapping index
5. Krishnan et al. [16]	1998	Experimental	Got average value of Young's modulus as 1.25 TPa
6. Yu et al. [17]	2000	Experimental (testing under tension)	*Y* value measured as 0.32–1.47 TPa and failure strength 13–52 GPa
7. Ozaki et al. [18]	2000	Quantum mechanical calculation	Failure stresses were found to be more than 100 GPa
8. Belyschko et al. [19]	2002	Atomistic simulation	Failure stress varies from 93.5 GPa and failure strain from 15.8% to 18.7%
9. Demczyk et al. [20]	2002	Experimental (pull and bend test)	*Y* value-0.91 TPa, Tensile strength 150 ± 45 GPa
10. Troya et al. [21]	2003	Quantum mechanical studies	*Y* values obtained in different methods as 0.82 TPa, 1.4 TPa and 1.16 TPa. Also observed the decreasing effect of failure strain on increasing number of SW defects
11. Chandra et al. [22]	2004	Theoretical measurement of stress in three different way	Got *Y* value around 1 TPa and Stiffness of defects reduces by about 30–50% by the presence of SW defect
12. Lu and Bhattacharya [23]	2005	Atomistic simulation	Randomly occurring defects can have significant effects on the mechanical properties and fracture process of the CNTs
13. Song et al. [24]	2006	A hybrid atomistic/continuum model	Bond breakage starts after the SW transformation, and failure strain 13%
14. Tserpes and Papanikos [25]	2007	MD simulation	SW serves as nucleation site for fracture. Reduction of failure stress by 18–25% and failure strain by 30–41% by the inclusion of defect
15. Richard et al. [26]	2007	Tight binding MD simulation	*Y* value 1.1 TPa, Decreasing effect of defects on the mechanical properties of CNTs
16. Pozrikidis [27]	2008	MD simulation	Studied the effects of circumferential as well inclined SW defects
17. Tunvir et al. [28]	2008	Classical MD simulation	Studied the effect of two vacancy and two SW defects with varying positions
18. Xiao et al. [29]	2009	Finite bond element model	Predicted fracture and progressive failure of grapheme sheet and CNTs. Noticed considerable change in failure stress incorporating defects

loads. Due to a cut-off function present in this potential, the pair potential only includes the contribution of the nearest neighbors.

On the other hand, Tight-Binding [32] Molecular Dynamics (TBMD) uses certain features from ab initio method and some features from molecular dynamics method. MD method treats atoms or molecules as the building blocks and finds their co-ordinates or momenta following Newtonian mechanics. The basic of ab initio method is to find out the exact solution of the Schrödinger equation. Assumptions and approximations are made to get the exact solution. In Tight-Binding approximation, the lattice sites are treated independently by assuming the atomic orbital to be very small beyond the lattice constant.

Using the potentials, MD simulation is carried out on a (5, 0) SWNT of length 21.3 Å and radius 1.96 Å (i.e. aspect ratio 10.87). We have taken 5 repeated units of the original building block of a (5, 0) SWNT which contains 100 atoms. Though the SWNT under consideration has a small length, having an aspect ratio greater than 10, the results will not be hampered by any end effect. Keeping one end fixed, stress is applied on the other end of the tube. Berendsen thermostat [33] is used to allow small changes in the velocities of the atoms such that temperature of the system reaches a certain value. Temperature is controlled by the thermostat to set at 300 K. Stress was calculated from the energy value according to the relation $\sigma = 1/A\ (dE/d\varepsilon)$ where σ is the stress, A is the area of the annular cross-section of the tube and $(dE/d\varepsilon)$ is the slope of the energy–strain curve. ε represents the strain. Area of the annular cross-section of the tube is found as $A = 2\pi r\delta r$ where r is the radius of the tube and δr, its wall thickness. We have taken δr as 0.34 nm and the Young's modulus (Y) was found from the slope of the linear portion of the curve.

3. Results and discussion

Results of the MD simulations show a scattering of data in all respects. For 1 and 2 defects, Young's modulus, failure stress and ductility show different values. Energies increase for defective tubes. That means, energy is required for the formation of Stone–Wales defects. At first, energies for slightly increasing strain values

دریافت فوری ← متن کامل مقاله

ISIArticles
مرجع مقالات تخصصی ایران

✓ امکان دانلود نسخه تمام متن مقالات انگلیسی
✓ امکان دانلود نسخه ترجمه شده مقالات
✓ پذیرش سفارش ترجمه تخصصی
✓ امکان جستجو در آرشیو جامعی از صدها موضوع و هزاران مقاله
✓ امکان دانلود رایگان ۲ صفحه اول هر مقاله
✓ امکان پرداخت اینترنتی با کلیه کارت های عضو شتاب
✓ دانلود فوری مقاله پس از پرداخت آنلاین
✓ پشتیبانی کامل خرید با بهره مندی از سیستم هوشمند رهگیری سفارشات