Composites: Part B 56 (2014) 435–449

Contents lists available at ScienceDirect

Composites: Part B

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

On the modeling of carbon nanotubes: A critical review

Roham Rafiee *, Reza Maleki Moghadam

Composites Research Laboratory, Faculty of New Sciences & Technologies, University of Tehran, End of The North Karegar St., Tehran 1439955941, Iran

ARTICLE INFO

Article history:
Received 11 February 2013
Received in revised form 10 May 2013
Accepted 12 August 2013
Available online 22 August 2013

Keywords:
A. Nano-structures
B. Mechanical properties
C. Computational modeling

ABSTRACT

A comprehensive review is conducted on the modeling and simulation of isolated carbon nanotubes (CNTs) concentrating on all mechanical, buckling, vibrational and thermal properties. Three different approaches consisting of atomistic modeling, continuum modeling and nano-scale continuum modeling are firstly explained and their applications toward understanding behavior of CNTs are discussed. Different investigations available in literature focusing on mentioned behaviors are reviewed and their results are compared to show the applicability and efficiency of employed/developed technique. Taking into account both runtime and accuracy of modeling, advantages and disadvantages of introduced methods are nominated and analyzed.

1. Introduction

In recent years, carbon nanotubes (CNTs) have received significant interests among scientists because of their unique properties. CNTs have a wide range of potentials for engineering applications due to their exceptional mechanical, physical, electrical properties and geometrical characteristics consisting of small diameter and high aspect ratio. It has shown that dispersion of a few weight percentages of nanotubes in a matrix dramatically increase mechanical, thermal and electrical properties of composite materials [1–7]. CNTs can be categorized as single-walled (SWCNT) and multi-walled (MWCNT) in terms of constitutive walls. SWCNTs have the higher specific stiffness and strength compared to those of MWCNTs [8]. Development of CNT-based structures and devices requires a good understanding of CNT's properties. Because of the huge cost and technological difficulties associated with experimental analysis at the scale of nano, researchers are encouraged to employ computational methods for simulating the behavior of nanostructures like CNTs from different mechanical, thermal and electrical points of view. The main objective of this paper is to review the available computational techniques for predicting mechanical behavior of CNT in literature. Different methods which have been employed in the past decades are introduced and then corresponding pros and cons are analyzed.

2. CNT nanostructure

Each wall of CNT can be imaginary generated by rolling up a graphene sheet into a seamless tube with a constant radius [9]. The structure of a CNT is defined by its chiral vector and chiral angle [10]. The chiral vectors $(n,0)$ and (n,m) represent "zigzag" (Z) and "armchair" (A) CNT configurations, respectively which is indicated by Eq. (1) including basis vectors $\overrightarrow{a_1}$ and $\overrightarrow{a_2}$. Defining the twist of a tube, the chiral angle varies between 0° and 30° [11]. Fig. 1 shows chiral index and different CNTs.

$$\overrightarrow{C_h} = n\overrightarrow{a_1} + m\overrightarrow{a_2} \tag{1}$$

3. Modeling techniques

The theoretical efforts in modeling CNT behavior can be categorized in three categories as atomistic modeling, continuum modeling and nano-scale continuum modeling which are elaborated subsequently. Constructed models for CNT employing aforementioned approaches are shown in Fig. 2.

3.1. Atomistic modeling

Atomistic modeling predicts the positions of atoms based on interactive forces and boundary conditions [12]. This information is required to solve Schrodinger wave equation for obtaining chemical information on materials. Atomistic modeling techniques can be classified into three main categories, namely the molecular dynamics (MD), Monte Carlo (MC) and *ab initio* approaches. Other atomistic modeling techniques such as tight bonding molecular dynamics (TBMD) [13], local density (LD), density functional theory (DFT) [14], Morse potential function model [15], and modified Morse potential function model [16] were also applied later on. The atomistic modeling approaches for predicting Young's

* Corresponding author. Fax: +98 21 88617087.
E-mail address: Roham.Rafiee@ut.ac.ir (R. Rafiee).

1359-8368/$ - see front matter © 2013 Elsevier Ltd. All rights reserved.
http://dx.doi.org/10.1016/j.compositesb.2013.08.037

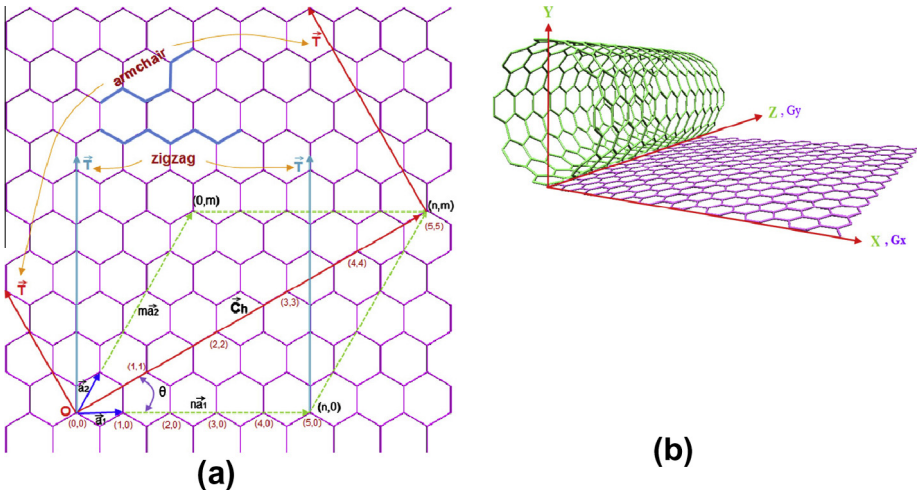

Fig. 1. Graphene sheet structure of a SWCNT: (a) Nano tube parameters and (b) rolling of planar lattice structure into CNT.

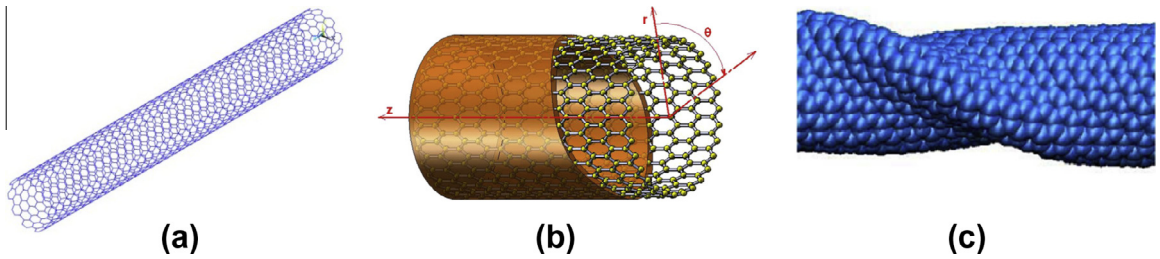

Fig. 2. Constructed models of CNT using: (a) Nano-scale continuum mechanics, (b) continuum modeling using shell model and (c) atomistic modeling techniques.

modulus of carbon nanotubes were comprehensively reviewed by Shokrieh and Rafiee [17].

The first technique used for simulating the behaviors of CNTs and CNT's allotropes was molecular dynamic (MD) method [18–21]. This method uses realistic many-body inter-atomic potential functions (force fields) to calculate the total energy of a system of particles. When the total potential energy and force fields of a system are obtained, the realistic calculations of the behavior and subsequently, the properties of a system of atoms and molecules can be acquired. Although the main aspect of both MD simulations and MC methods is geared down to second Newton's law, MD methods are deterministic approaches, while MC methods are stochastic ones. Meanwhile, the *ab initio* techniques are accurate methods which are based on an accurate solution of the Schrödinger equation. Furthermore the *ab initio* techniques are potential-free methods wherein the atoms forces are determined by electronic structure calculations progressively. In contrast, the MD and MC methods depend on the potentials that the forces acting on atoms are acquired by differentiating interatomic potential functions [17]. Zhang et al. [22] studied the impression of polymer wrapped SWCNT's dispersion on their load transfer using MD simulations. The density functional based tight binding method was exploited by Ganji et al. [23] to study the effect of curvature on armchair SWCNT's atoms average energy and Young's modulus. It is generally accepted that MD simulations provide good predictions of the mechanical properties of CNTs under external forces. However, MD simulations take long times to produce the results and consumes a large amount of computational resources, especially when dealing with long and multi-walled CNTs incorporating a large number of atoms.

3.2. Continuum modeling

Continuum mechanics-based models are utilized by many engineers to investigate properties of CNTs. The basic assumption in these theories is that a CNT can be modeled as a continuum structure which has continuous distributions of mass, stiffness, etc. So, the lattice structure of CNT is simply neglected in continuum modeling and it is replaced with a continuum medium. It is important to carefully investigate the validity of continuum mechanics approaches for modeling CNTs which the real discrete nano-structure of CNT is replaced with a continuum one (see Fig. 2b). The continuum modeling can be either accomplished analytical or numerically representing FEM.

Different researchers applied continuum shell models to study the CNT properties. Yakobson et al. [24–27] showed similarities between MD simulation of CNTs and macroscopic shell model. It has shown that mechanical properties of CNTs were strongly dependent on helicity and atomic structure of the tubes and obviously the curvature and chirality effects on the mechanical behavior of CNTs cannot be captured in an isotropic shell model, due to neglecting the discrete nature of the CNT geometry in this method. Chang [28] used an anisotropic shell model to study mechanical properties of single-walled carbon nanotubes, unlike common shell model for SWCNTs which is constructed as an isotropic continuum shell with constant elastic properties, the MBASM model can predict the chirality induced anisotropic effects on some mechanical behaviors of CNTs by incorporating molecular and continuum mechanics solutions. The applicability and limitations of shell models have been extensively discussed by some researchers [29,30]. Silvestre and co-workers [31–34] have shown that shallow