Computational Materials Science 101 (2015) 260–266

Contents lists available at ScienceDirect

Computational Materials Science

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

Characterizing the mechanical properties of carbon nanocones using an accurate spring-mass model

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ARTICLE INFO

Article history:
Received 25 February 2014
Received in revised form 24 January 2015
Accepted 1 February 2015

Keywords:
Carbon nanocones
Finite element
Spring-mass model
Mechanical properties

ABSTRACT

A three-dimensional finite element (FE) formulation based on a spring-mass model is presented to investigate the mechanical properties of single-walled carbon nanocones (SWCNCs). The rotational spring elements together with longitudinal ones are employed for modeling the covalent bond between the carbon atoms, and the carbon atoms are modeled by mass elements. Analytical expressions for Young's and shear moduli of SWCNCs with five feasible apex angles are obtained in terms of axial and torsion loads, respectively. The effects of geometrical parameters on the mechanical properties of SWCNCs are investigated. It is found that the apex angle of SWCNCs has a significant influence on their Young's and shear moduli. Moreover, in contrast to the results of similar works in the literature, the present results reveal that the length and small radius of nanocones do not play a major role in their mechanical properties. It is shown that with increasing small radius, Young's modulus slightly increases. To assess the accuracy of the developed FE formulation, molecular dynamics simulations are also conducted.

1. Introduction

After Iijima's paper about carbon nanotubes (CNTs) [1], a great deal of attention has been paid to study different features of these nanostructures due to their novel electrical, mechanical, physical and chemical properties. Because of the difficulties in the nanoscale experimentation, the theoretical modeling of nanostructures has been developed. There have been several methods for analyzing the mechanical behavior of CNTs, including molecular dynamics (MD) simulations, molecular mechanics (MM) approach and continuum mechanics theories [2–5]. Liew et al. [4] investigated buckling behavior of single-walled carbon nanotubes (SWCNTs) and multi-walled carbon nanotubes (MWCNTs) under axial compression by using the MD simulations. Employing a Timoshenko beam model, Wang et al. [5] studied the free vibration behavior of MWCNTs.

Moreover, conical nanostructures have attracted the attention of researchers owing to their special geometrical shape [6–8]. Carbon nanocones (CNCs) as the most favorable kinds of conical nanostructures were discovered in 1994 [9]. Due to the sharp-tip structure of CNCs, they can be utilized to achieve specific mechanical properties. These nanostructures can also be used in scanning tunneling probe, atomic force microscopy and field emission devices [10,11]. Although the first research into CNCs was almost simultaneous with the discovery of CNTs, CNCs were not as attractive as CNTs in research community and only some basic properties of them were investigated. Ge and Sattler [9] predicted that there are five feasible configurations for nanocones and the apex angle of CNCs is not arbitrary. Additionally, SWCNC was fabricated by Iijima et al. [12]. Klein [13] presented the existence of five positive curvatures and eight different types of cones, depending on the arrangement of the hexagons on the cone. Eksioglu and Nadarajah [14] investigated the structure of CNCs using molecular models and structural analyses. Utilizing transmission electron microscopy (TEM), synchrotron X-ray and electron diffraction, Naess et al. [15] investigated morphologies of the CNCs with different apex angles.

The mechanical behavior of CNCs can be investigated through the use of the theoretical models that have been used to study CNTs. Wei and Srivastava [16] suggested a general analytical solution for Young's modulus of a SWCNC. Wei et al. [17] expressed that the mechanical properties of CNCs such as Young's modulus depend on their apex angles, height and small radius. They also measured Young's modulus of this nanostructure and concluded that Young's modulus of CNCs varies from 0.29 to 0.73 TPa. Furthermore, Firouz-Abadi et al. [18] combined a shell model with the nonlocal continuum theory to derive the nanocones governing

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http://dx.doi.org/10.1016/j.commatsci.2015.02.001
0927-0256/

equations of motion. They also studied the free vibration characteristics of CNCs. In another work, Firouz-Abadi et al. [19] employed the same approach to derive the governing equations of motion with considering the geometric non-linearity by using the von-Karman strain tensor. The stability of nanocones was studied by Mustapha and Zhong [20] employing a tapered beam model. Using the MD simulations, Tsai and Fang [21] presented the nucleation, thermal stability and nanomechanical properties of the CNCs. They compared their results with the ones obtained for CNTs and showed the dependence of CNCs properties on their apex angles. The structural parameters and elastic properties of SWCNCs were studied by Yan et al. [22] via a higher-order continuum theory. In their study, all five types of CNCs were chosen to investigate the effect of the conical angle on the mechanical properties of CNC.

Amongst the theoretical methods that applied to study the mechanical behavior of nanostructures, finite element method (FEM) has been used extensively to investigate the mechanical response of graphene sheets, CNTs and CNCs. For example, employing a FE approach, Pantano et al. [23] modeled the deformation of CNTs. Utilizing a three-dimensional FE model, Tserpes and Papanikos [24] specified Young's modulus and shear modulus of armchair, zigzag and chiral SWCNTs. The mechanical properties of SWCNTs were investigated by Giannopoulos et al. [25] using a spring-based FE approach. In another work, the resonant frequencies of the CNTs were calculated by Yun and Park [26] to utilize in nanoscale mass sensing. Mahmoudinezhad et al. [27] developed an accurate spring-mass FE formulation to estimate Young's and shear moduli of SWCNTs. They employed a rotational spring for simulating the bond angle bending and out-of-plane angle torsion interaction. In another work, Mahmoudinezhad and Ansari [28] investigated the vibrational behavior of circular and square single-layered graphene sheets using a spring-mass FE model. Additionally, Mahmoudinezhad et al. [29] studied vibration behavior of SWCNTs using the same method. They achieved two helpful relations for approximating the fundamental frequency of relatively large carbon nanotubes. A modal analysis of SWCNTs and SWCNCs was performed by Lee and Lee [30] utilizing ANSYS software. They calculated the natural frequencies and mode shapes of these nanostructures. The elastic and buckling behaviors of CNCs with different geometrical parameters were investigated by Fakhrabadi et al. [31] using the molecular mechanics-based FEM. In their work, the elastic modulus and compressive forces of the axial buckling for CNCs with different boundary conditions were reported.

In this paper, based on the spring-mass FE method, an accurate spring-mass model is developed to evaluate the mechanical properties of SWCNCs with different geometrical parameters. A rotational spring is employed for the simulation of the bond angle bending and out-of-plane angle torsion interactions. Using the proposed method, analytical formulas for Young's and shear moduli of these nanostructures are derived and graphically illustrated. It should be noted the analytical expression of shear modulus is proposed for the first time. The results indicate that contrary to apex angle, the effects of length and small radius on the mechanical properties of nanocones are insignificant.

2. Geometry of carbon nanocones

In order to obtain coordinates of carbon nanocones, we need to roll up a circular sector of graphene sheet into a conical shape. Therefore, an appropriate mapping is needed to transform coordinates of a two-dimensional plane into a three-dimensional structure (Fig. 1). Choosing the center of a hexagonal unit cell as the center of circular sector of graphene provides a rotational symmetry of order six (see Fig. 2a). Therefore, we have five options to select a sector of graphene for initial shape of mapping process by

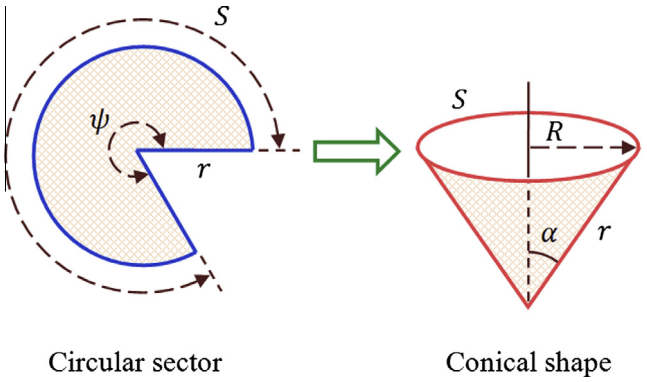

Fig. 1. Transforming a circular sector to a conical shape.

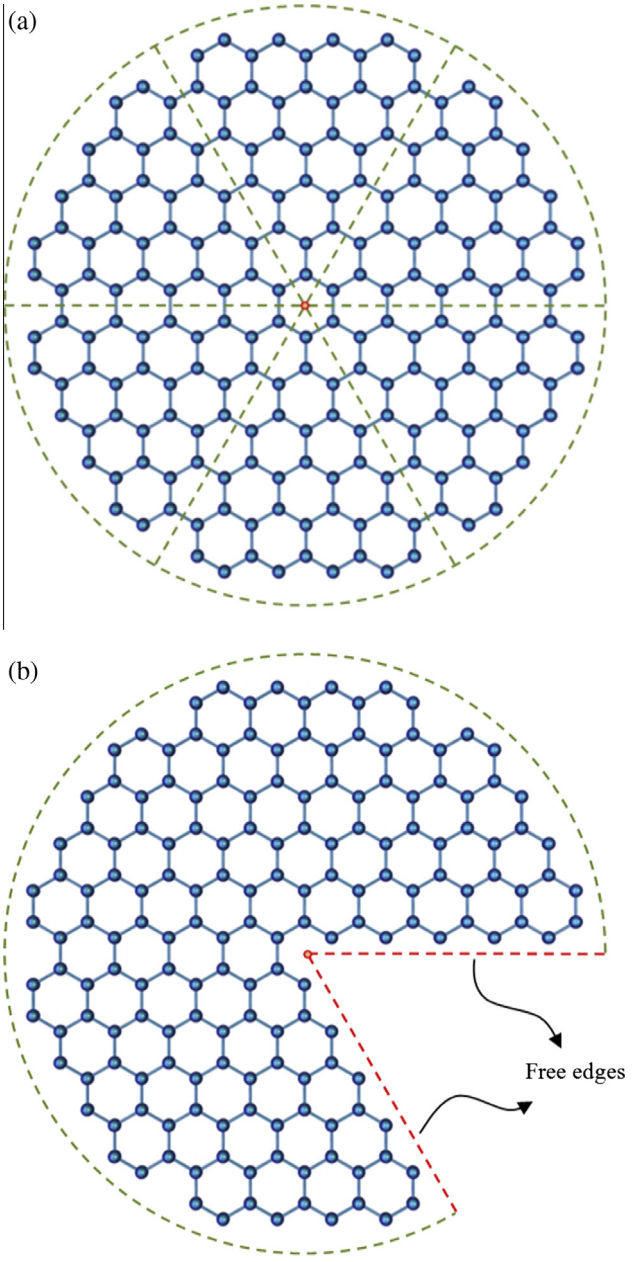

Fig. 2. (a) A circular graphene sheet with rotational symmetry of order six. (b) Initial shape of mapping process.