



An accurate spring-mass finite element model for vibration analysis of single-walled carbon nanotubes



E. Mahmoudinezhad, R. Ansari*, A. Basti, M. Hemmatnezhad

Department of Mechanical Engineering, University of Guilan, P.O. Box 3756, Rasht, Iran

ARTICLE INFO

Article history:

Received 5 July 2012

Received in revised form 17 October 2013

Accepted 25 November 2013

Available online 19 January 2014

Keywords:

Carbon nanotubes

Vibration frequencies

Spring mass model

Finite element method

Interatomic potential

ABSTRACT

An accurate spring-mass model, in the context of a three-dimensional finite element formulation, is developed for investigating the vibrational characteristics of single-walled carbon nanotubes (SWCNTs). Atoms are replaced by lumped mass elements at their locations and appropriate spring-type elements are defined as interconnections between the atoms in order to simulate the interatomic interactions. The effect of out of plane angle variation energy is incorporated into the model. The obtained results for the fundamental frequency of single-walled carbon nanotubes of various kinds are graphically illustrated. The influences of some commonly-used boundary conditions and changes in the nanotube geometrical parameters on vibration frequencies are examined. The numerical results show good agreement with other published results in the literature. Also, some novel relations are deduced which can be more useful in predicting the fundamental frequency of SWCNTs with great number of atoms.

© 2013 Elsevier B.V. All rights reserved.

1. Introduction

The number of publications on carbon nanotubes (CNTs) has increasingly grown since the appearance of Iijima's landmark paper [1] in 1991. Their novel and superior electronic, mechanical and other physical and chemical properties have attracted great attention of many researchers in the globe. These unique properties have provided CNTs with numerous potential applications in nanoelectronics, nanodevices, nanocomposites and so on [2–9]. CNTs have very large Young modulus in their axial direction which is measured near to 1 TPa. Also, their tensile strength is about 100 times higher than that of steel at one-sixth of the weight [10].

In recent years, vibrational characteristics of CNTs have been widely studied using several methods such as experimental techniques [11–15], molecular dynamics simulations [16,17], molecular structural mechanics approach (MSMA) [18–24] and continuum mechanics theories [25–35]. In molecular dynamics simulations, atoms are considered as particles interacting to each other through several types of potential fields. Although molecular dynamics simulations generate abundant results for understanding the behavior of structures, but the major concern about this method is the limitation of working with atomic systems in the scale of nanometer and this leads to time consuming and complicated computational efforts. In MSMA atoms and bonds are considered as joints and beams, respectively. Based on the continuum

mechanics theory, each nanotube is modeled as a single continuous beam or shell. Then, the governing vibration equations of beams and shells are used for investigating the vibrational characteristics of nanotubes. However, MSMA gives more accurate models for CNTs rather than the continuum mechanics, but the former is slightly more time consuming. Amongst the aforementioned methods, continuum mechanics due to its simplicity has allocated a remarkable portion of publications conducted on the vibration of CNTs. Recently, a comprehensive review was published by Gibson et al. [10] on the vibrations of CNTs and their composites. The number of publications conducted on the comprehensive study of the vibrational behavior of SWCNTs is scarce and less works can be seen in the literature dealing with the general vibration spectra of SWCNTs with armchair and zigzag structures and various aspect ratios.

Using MSMA, Behfar and Naghdabadi [36] investigated the vibration of embedded multilayered graphene sheet. However, they did not include the cylindrical zigzag, armchair or chiral nanotubes in their study. Based on MSMA, Hashemnia et al. [37] implemented the finite element method to determine the fundamental frequencies and their corresponding modes for graphene sheets and two types of nanotubes i.e., zigzag and armchair. In their analysis, carbon atoms and interatomic bonds are considered as concentrated masses (joints) and beams, respectively. Then, the equivalent space frame can be achieved by setting equality between strain energies of each element and potential energies of each bond. Georgantzinos et al. [38] presented a linear spring-based element formulation for computation of vibrational

* Corresponding author. Tel./fax: +98 131 6690276.

E-mail address: r_ansari@guilan.ac.ir (R. Ansari).

characteristics of SWCNTs. The major concern about their model is the consideration of a linear spring between two bonds for calculating the potential energies due to the bond angle bending. For example, when atom moves along one of its bonds, the model given by [38] does not give the real potential energy variation of the structure. Chowdhury et al. [39] investigated the vibrational characteristics of armchair and zigzag SWCNTs using the MSMA. They used the universal force field potential which is in accordance with the formulation given in [40]. Based on a modified molecular structural mechanics model, Cheng et al. [41] studied the RBM (radial breathing mode) frequencies and mode shapes of different carbon CNTs. They indicated that asymmetric, non-purely radial RBM modes are observed in the chiral CNTs mainly due to their non-axisymmetric atomic structure.

In this work, a spring-mass finite element formulation [42,43] is employed for investigating the fundamental frequency of zigzag and armchair SWCNTs. A rotational spring is implemented for simulating the bond angle bending and out of plane angle torsion interactions which remove the overestimation of the natural frequencies caused through using continuum mechanics theories, structural mechanics using beam elements and spring-mass models using linear springs. Further, the influences of some commonly used boundary conditions and changes in the nanotube's geometrical parameters on the vibration frequencies are examined. Some new graphical illustrations are made and two proportional relations are deduced which can be more useful in predicting the fundamental frequency of SWCNTs with high dimensions.

2. Interatomic potential energies

The major concern about the molecular mechanics calculations is the definition of the interaction forces between individual atoms. The total potential energy of atoms is used for defining this force field. Neglecting the effect of the electrostatic interaction, the total potential energy which is the summation of energies emerged due to the different interatomic interactions, can be described by the following relation:

$$E = \sum E_r + \sum E_\theta + \sum E_\phi + \sum E_\omega + \sum E_{vdW} \quad (1)$$

where E_r , E_θ , E_ϕ , E_ω are energies due to the bond stretching, angle variation, dihedral angle torsion and out of plane torsion, respectively, and E_{vdW} stands for the Van der Waals interactions. For sake of simplicity, one can describe the potential energy by the harmonic approximation. Therefore, the potential energy terms corresponding to dihedral angle torsion and out of plane torsion can be merged together and an equivalent energy term is replaced instead, i.e.,

$$E_r = \frac{1}{2} k_r (\Delta r)^2 \quad (2)$$

$$E_\theta = \frac{1}{2} k_\theta (\Delta \theta)^2 \quad (3)$$

$$E_\beta = E_\phi + E_\omega = \frac{1}{2} k_\beta (\Delta \beta)^2 \quad (4)$$

where k_r , k_θ , k_β stand for the bond stretching force constant, bond angle variation force constant and out of plane angle variation resistance, respectively. In the above equations, the terms Δr , $\Delta \theta$, $\Delta \beta$ and represent the increment in bond length, changes in bond and out of plane angles, respectively.

3. Finite element modeling

Writing the stiffness matrix of the longitudinal spring (the C–C bonds) will be performed in a similar manner as space trusses as

$$[k]^i = k_r \begin{bmatrix} l_i^2 & l_i m_i & l_i n_i & -l_i^2 & -l_i m_i & -l_i n_i \\ l_i m_i & m_i^2 & m_i n_i & -l_i m_i & -m_i^2 & m_i n_i \\ l_i n_i & m_i n_i & n_i^2 & -l_i n_i & -m_i n_i & -n_i^2 \\ -l_i^2 & -l_i m_i & -l_i n_i & l_i^2 & l_i m_i & l_i n_i \\ -l_i m_i & -m_i^2 & m_i n_i & l_i m_i & m_i^2 & m_i n_i \\ -l_i n_i & m_i n_i & -n_i^2 & l_i n_i & m_i n_i & n_i^2 \end{bmatrix} \quad (5)$$

here l_i , m_i and n_i stand for the direction cosines of the bond i and the three coordinate axes.

In the case of rotational springs we must write the potential energy due to changes in positions of involved atoms with that angle (see Fig. 1). This is due to the fact that the coordinates of three involved atoms changes as this angle changes. Therefore the corresponding potential energy is given as below

$$U_\theta = \frac{1}{2} k_\theta (d\theta^2) \quad (6)$$

If we write the potential energy variation due to this angle change by using the Cartesian coordinates of the nodes, the stiffness matrix components of the rotational spring can be successfully achieved by differentiating from this potential energy according to Castigliano's theorem. Since three nodes are involved with this angle, the size of stiffness matrix will be 6×6 in the case of two-dimensional and 9×9 in three-dimensional one. For sake of simplicity, the corresponding relations for two-dimensional case are considered here.

The net change between two bonds angle is identical to the difference between the changes in the two bond angles as

$$d\theta = d\theta_1 - d\theta_2 \quad (7)$$

where $d\theta_1$ and $d\theta_2$ are introduced as

$$d\theta_1 \cong \sin(d\theta_1) = \left| \frac{\vec{r}_1 \times \vec{r}'_1}{l_e^2} \right| \quad (8)$$

$$d\theta_2 \cong \sin(d\theta_2) = \left| \frac{\vec{r}_2 \times \vec{r}'_2}{l_e^2} \right| \quad (9)$$

where r_1 and r_2 vectors are the bonds before deflection and can be written as follows:

$$r_1 = l e_1 (l_1 \hat{i} + m_1 \hat{j}) \quad (10)$$

$$r_2 = l e_2 (l_2 \hat{i} + m_2 \hat{j}) \quad (11)$$

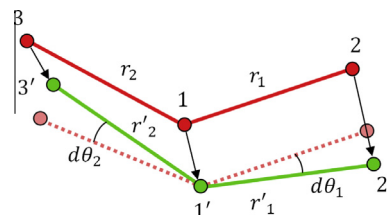


Fig. 1. Displacement of atoms with angle variations (green lines show the bond status after deflection and black arrows are related to displacement vectors). (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

Download English Version:

<https://daneshyari.com/en/article/1560982>

Download Persian Version:

<https://daneshyari.com/article/1560982>

[Daneshyari.com](https://daneshyari.com)