Computational Materials Science 122 (2016) 11–21

Contents lists available at ScienceDirect

Computational Materials Science

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

The effects of connecting region length on the natural frequencies of straight and non-straight hetero-junction carbon nanotubes

Mostafa Mohammadian [a], Mohammad Hossein Abolbashari [b,*], Seyed Mahmoud Hosseini [c]

[a] Department of Mechanical Engineering, Faculty of Engineering, Ferdowsi University of Mashhad, P.O. Box 91775-1111, Mashhad, Iran
[b] Department of Mechanical Engineering, Lean Production Engineering Research Center, Ferdowsi University of Mashhad, P.O. Box 91775-1111, Mashhad, Iran
[c] Industrial Engineering Department, Faculty of Engineering, Ferdowsi University of Mashhad, P.O. Box 91775-1111, Mashhad, Iran

ARTICLE INFO

Article history:
Received 15 February 2016
Received in revised form 1 May 2016
Accepted 7 May 2016

Keywords:
Hetero-junction carbon nanotubes
Vibrational behavior
Molecular mechanics
Finite element method

ABSTRACT

In the present study, the vibrational properties of straight and non-straight hetero-junction carbon nanotubes (HJCNTs) are investigated. The molecular mechanics technique in combination with the finite element method is applied to obtain the first four natural frequencies as well as the corresponding mode shapes. The effects of connecting region length on the frequencies of straight and non-straight structures with clamp-clamp and clamp-free boundary conditions (BCs) are discussed in details. The results show that for the clamp-free BCs, the first and second frequencies increase with increasing the connecting length whereas the third and fourth ones decrease. Also, for the clamp-clamp BCs, increasing the connecting length leads to decrement in the first two frequencies while the changes of the second two frequencies depend on the total length of the structure. Moreover, for the clamp-clamp BCs, the mode shapes are affected by the total length of the structures. Finally, to avoid resonance and its damage in dynamic applications, for some modes of excitation appropriate structures are proposed.

1. Introduction

Carbon nanotubes have been an area of interest since 1991s, when they were first discovered by Iijima [1]. Afterward, several studies regarding the investigation of mechanical, electrical, chemical, physical and thermal properties of these nanostructures have been carried out by various researchers. Overall, from the mechanical point of view, the researches show considerable promise of CNTs superior specifications such as light weight structures, high elastic modulus and stiffness [2,3]. These nanostructures can be utilized as oscillators, vibrational sensors and electromechanical resonators. Hence, studying their vibrational properties provides important and useful results.

Applying the experimental methodology to investigate the mechanical and specially vibrational properties of such nanotubes is often expensive. Therefore, simulation approaches are of great interest. Many well-known simulation methods such as molecular dynamics (MD), ab initio, Monte Carlo (MC) and molecular mechanics (MM) have been used by several scientists [4–6].

In the current study, the MM method is applied to investigate the vibrational properties of a special kind of carbon nanostructure. The focus of the following literature review is also on the application of the MM method in vibrational characterization of CNTs.

Li and Chou [7] utilized the MM technique to study the vibrational behavior of CNTs. They considered the CNTs as nanomechanical resonators with the clamp-free and clamp-clamp boundary conditions (BCs). Also, they found that the fundamental frequency can be altered in the range of 10 GHz–1.5 THz. The modified MM method was proposed by Lu et al. [8] to analyze the dynamic characteristics of cantilevered CNTs. They confirmed that the frequency significantly depends on the length and diameter to the extent that the frequency reaches to the GHz level for small diameter. Hosseini and Majzoobi [9] directed a numerical study to investigate the vibrational response of zigzag and armchair CNTs using the finite element (FE) methodology. To consider the covalent force between carbon atoms, they used the beam element in their FE simulations. The obtained results showed that for CNTs with the same diameter, the frequency decreases with the length increment. Also, they concluded that frequencies of CNTs with chirality of $(m,0)$ and (m,m) are close to each other at the first two modes, whereas they are different for the higher modes. Fundamental frequency of two kinds of nanostructures, i.e. CNTs and grapheme sheet were reported by Hashemnia et al. [10] in which the CNTs were considered as space frames structures and MM method was used for the FE formulation. They showed that fundamental frequency reduces with increasing the aspect ratio. Hence, they suggested to utilize CNTs

* Corresponding author.
E-mail addresses: mo.mohammadyan@gmail.com (M. Mohammadian), abolbash@um.ac.ir (M.H. Abolbashari), sm_hoseini@yahoo.com (S.M. Hosseini).

http://dx.doi.org/10.1016/j.commatsci.2016.05.005
0927-0256/

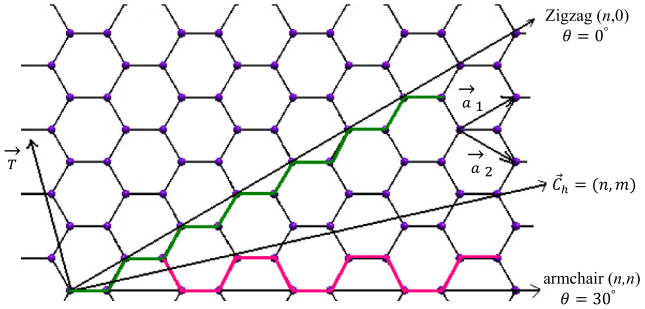

Fig. 1. The chiral vector of a CNT.

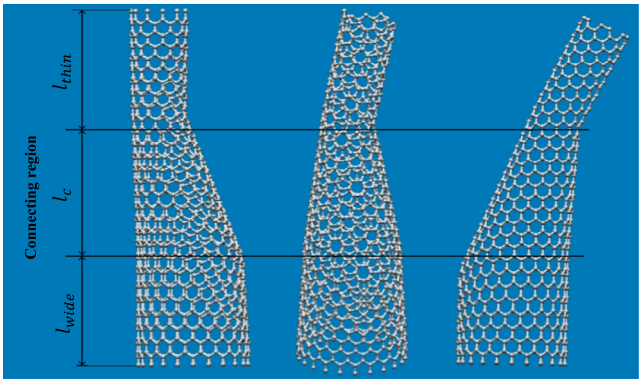

Fig. 2. A typical straight and non-straight HJCNTs.

Table 1
Molecular mechanics constants [11].

k_r	6.52e − 7 N nm^{-1}
k_θ	8.76e − 10 N nm rad^{-2}
k_φ	2.78e − 10 N nm rad^{-2}

with the lower aspect ratio for dynamics applications. Moreover, they reported that the first frequency of CNTs is higher than that of graphene sheets. In another research work, the first ten natural frequencies and the corresponding mode shapes of zigzag and armchair CNTs were obtained by Sakhaee-pour et al. [11]. They employed beam elements to consider the covalent bond between carbon atoms and the MM technique to obtain the elements properties. Also, using the atomistic results and the statistical nonlinear regression model, they developed an equation to estimate the frequencies of CNTs with different BCs and geometries. Chowdhury et al. [12] investigated the vibration of CNTs using the MM method. The universal force field potential was applied in their work. They

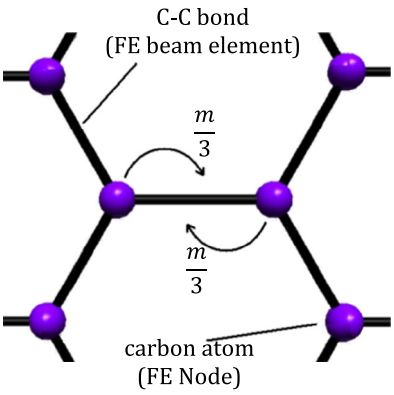

Fig. 3. A schematic of beam elements and nodes for presentation the C–C bonds and carbon atoms in FE modeling.

studied the first five natural frequencies of four types of zigzag and three types of armchair CNTs. The results were presented for various chiralities, BCs and aspect ratios. Fakhrabadi et al. [13] employed the MM method to study the natural frequencies and the corresponding mode shapes of the CNTs. The neural network method was used by them to predict the frequencies of unmodeled CNTs. In addition, the effect of twisting and distortion of cross section was discussed and it was found that, in various BCs, increasing the twisting angle decreases the frequencies. Also they illustrated that by increasing distortion ratio, the first, third and fifth frequencies decrease while the second and fourth ones increase.

Hetero-junction carbon nanotubes (HJCNTs) are relatively novel nanostructures which are constructed by connecting two CNTs with different diameters. These nanostructures can be constructed by predetermined temperature-mediated growth during catalytic vapor deposition (CVD) [14]. HJCNTs can be used as functional component in nanodevices [15], rectifying diodes [16], and switches. In addition, Arora and Sandler [17] reported the feasibility of them as nano-pores and nano-sieves in transport problems. For example, due to existence of constriction in their structure, they can filter the oxygen and nitrogen molecules. Moreover, researchers proposed some other applications such as blood vessels or flow sensors in the nano-measurement methods [4]. Axial vibration of HJs using nonlocal theory was investigated by Filiz and Aydogdu [18]. They used nonlocal constitutive relations of Eringen and studied the effects of chirality, length and diameter of corresponding carbon nanotubes in vibrational properties. Fakhrabadi et al. [4] applied the MM using FE method to obtain the vibrational properties of two and three connected CNTs. Different diameters and lengths as well as three various BCs were considered in their work. They found that increasing the length decreases the fundamental frequency. In another work, the buckling behaviors of

Table 2
The comparison between the obtained frequencies (GHz) in this study and other references.

Nano structure	Chirality	L (nm)	BCs	Mode 1		Mode 2		Mode 3		Mode 4		Ref. no.
				Present	Ref.	Present	Ref.	Present	Ref.	Present	Ref.	
CNT	(6,6)	10.58	C-F	30.96	31	30.96	31	184.44	183	184.44	183	[11]
	(6,6)	10.58	C-C	184.81	185	184.81	185	469	469	469	469	[11]
	(22,0)	13.9	C-F	34.42	34	34.42	34	195.58	193	195.58	193	[11]
	(22,0)	13.9	C-C	192	191	192	191	460.7	459	460.7	459	[11]
HJCNT	(8,8)–(14,14)	16.2	C-F	34.65	34.5	35.07	34.9	127.33	127	129.47	129	[4]
	(8,8)–(14,14)	16.2	C-C	126.16	126	128.7	129	332	335	341.32	344	[4]
	(5,5),(10,10)	15	C-F	30.5	27	30.9	–	105.4	–	107	–	[24]
	(9,0),(12,0)	15	C-F	19.79	20	19.93	–	93.238	–	94.9	–	[24]