Journal of Nano Research *Online: 2012-01-11*
ISSN: 1661-9897, Vol. 16, pp 153-160
doi:10.4028/www.scientific.net/JNanoR.16.153

Buckling Behaviour and Natural Frequency of Zigzag and Armchair Single-Walled Carbon Nanotubes

Moones Rahmandoust[1,a], Andreas Öchsner[1,b]

[1]Faculty of Mechanical Engineering, Universiti Teknologi Malaysia UTM 81310 Johor Bahru, Johor, Malaysia

[a]moones.r@gmail.com (corresponding author), [b]andreas.oechsner@gmail.com

Keywords: Finite element model; Carbon nanotube; resonance frequency; natural frequency; buckling; cantilever.

Abstract. In this study, single-walled carbon nanotubes were generated in their perfect state as finite element models in the MSC.Marc software. The buckling behaviour and resonant frequency modes of the two limiting cases of carbon nanotubes, i.e. the armchair and zigzag models, were studied. The obtained results were compared with the classical analytical solutions related to a similar continuum structure of a hollow cylinder. The buckling behaviour of single-walled carbon nanotubes under cantilever boundary conditions proved to be almost identical to the prediction of the classical Euler equation. Furthermore, there was very good agreement between the analytical and finite element results of the studied single-walled carbon nanotubes; though the achieved value of the first mode of frequency, obtained from the finite element results, was more accurate than the higher modes.

Introduction

Carbon nanotubes (CNTs) have attracted much attention as promising candidates in emerging new technologies as a result of their outstanding mechanical, electrical and thermal properties [1]. They are expected to influence many fields in terms of technology and industry. They will have applications in many diverse fields such as energy, signal processing, medicine, biotechnology, information technology, aerospace, agriculture, and environment [6]. These outstanding materials can be used as stand–alone nanomaterials or as reinforcements in composites for a wide variety of application. Therefore, several detailed studies have been conducted to explore different properties of carbon nanotubes.

Mechanical properties of carbon nanotubes have been characterised both experimentally and computationally. Molecular Dynamics (MD) and continuum mechanics techniques such as the Finite Element Method (FEM) are the two most commonly used computational approaches to study the behaviours of CNTs. These investigations focus each on different properties of CNTs, using different approaches. Properties such as Young's modulus, Poisson's ratio, shear modulus, buckling behaviour and resonance frequency of different CNTs and CNT–based nanocomposites under different conditions have been studied by different scientists all over the world [2, 6, 8–10].

Young's modulus of carbon nanotubes in their axial direction, as obtained from both experimental and computational investigations, is very high, i.e. about 1 TPa, while a Poisson's ratio around 0.05–0.28 was reported depending on the approach and the energy potential used [1–4]. Shear modulus of carbon nanotubes has also been evaluated by two types of tests, i.e. torsion and tensile

tests and it is reported to be in the range of 0.2 and 0.5 TPa which is considered a high shear modulus [1–4, 9]. As a result of the valuable mechanical properties of single-walled carbon nanotubes (SWCNTs), these materials have become specifically interesting for applications in nanomechanical devices and low–weight ultra-strong composite materials.

Buckling behaviour and natural resonance frequency of single- and multi-walled carbon nanotubes were also investigated by many scholars. Carbon nanotubes are very vulnerable to buckling as they are long and hollow structures. However, the results show that they are at the same time capable of retaining their buckling capacity and recover their elasticity [6, 9]. A brief review on the recent investigations about the buckling properties of CNTs has been published by Wang *et al.* [6].

The natural frequency of carbon nanotubes was also an important factor to be investigated. As a result of their small size, carbon nanotubes can make acceptable resonators in signal processing systems. The resonant frequency enhances as the size of the resonator decreases and higher resonance frequency is equal to higher sensibility [11].

Finite Element Modelling

The Atomic Structure. The atomic structure of nanotubes can be imagined as a graphene sheet that has been rolled into a tube. The thickness of the tube's wall is generally considered to be 0.34 nm, which is very close to that of a graphene sheet, i.e. 0.335 nm [4, 5, 7]. The hybridization of carbon atomic orbitals in the covalent bonding of carbon nanotubes is of type sp^2, in which each atom is joined to three other nearest neighbours in a hexagonal arrangement.

Carbon nanotubes can be single-walled, with a diameter in range of 0.4–3.0 nm; or they can consist of two to fifty coaxial tubes with an inter-layer spacing of 0.34 nm. The diameter of multi-walled carbon nanotubes generally ranges from 4 to 30 nm.

Tube chirality or helicity is the characteristic that is used to define the size of the carbon nanotube. The chiral vector $\overrightarrow{C_h}$, , also known as the roll-up vector, as is shown in Figure 1, is defined by the integers *n* and *m*; the number of steps along the unit vectors $\overrightarrow{a_1}$ and $\overrightarrow{a_2}$:

$$\overrightarrow{C_h} = n\overrightarrow{a_1} + m\overrightarrow{a_2} . \quad (1)$$

By rolling the graphene sheet in a way that the tip of the chiral vector $\overrightarrow{C_h}$ touches its tail, a (*m, n*) carbon nanotube can be visualised. The fundamental (*m, n*) carbon nanotube is classified into three main categories according to its chirality, i.e. zigzag, armchair and chiral.

For a chiral (*m, n*) tube in general, the integers *m* and *n* are not equal, i.e. $m \neq n$, whereas for zigzag and armchair tubes, the two limiting cases of twisting, the zigzag structure is formed when $m = 0$, and $m = n$ makes the armchair case. The latter two cases, shown in figure 1, are the symmetric carbon nanotubes but what is observed in practice is not generally as perfect as these idealised forms. There are many types of imperfections involved in real CNT structure and CNT-based composites that influence their mechanical properties [3, 12].

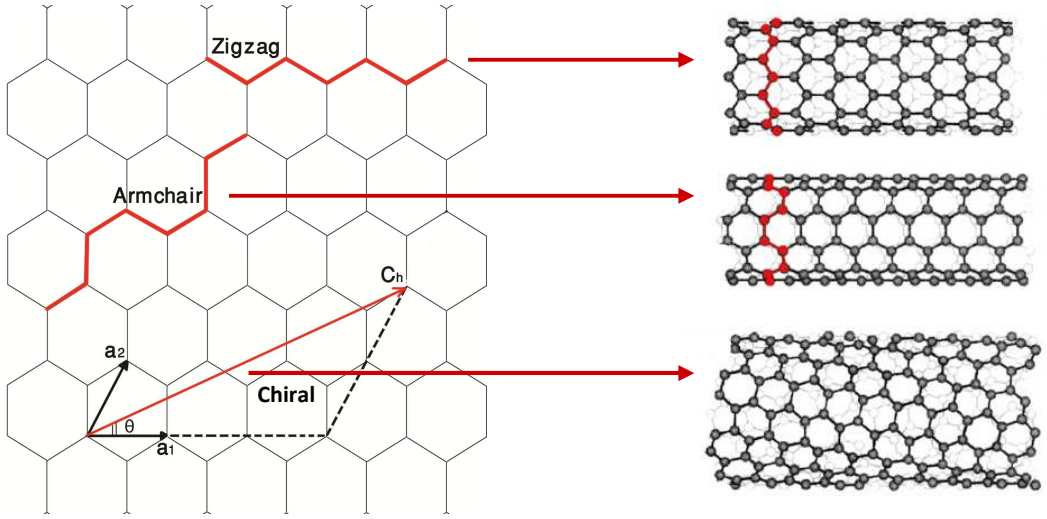

Figure 1. Schematic diagram showing zigzag, armchair and chiral carbon nanotubes.

FEM Model. As shown in Figure 2, each CNT is made up of a unit cells repeated and rotated to make the whole structure. Each carbon-carbon covalent bond is represented by an Euler-Bernoulli elastic beam element in the finite element program MSC.Marc. The unit cell is not allowed to bend on the covalent bonds, but it can bend on the joints, i.e. the carbon atoms' locations, to cover the tube's curvature.

The phenomenon of *buckling* is a kind of elastic instability in a structure that occurs under a certain compressive load. In the theory of elasticity, the critical buckling load of a structure, as defined in Eq. (2), i.e. the famous Euler formula of buckling load, depends on its shape and geometry, as well as its boundary conditions.

$$P_{cr} = \frac{n^2 \pi^2 E I}{(KL)^2}, \tag{2}$$

where P_{cr} is the critical buckling load, E is the structure's axial Young's modulus, K is the effective length constant and L is the length of the tube. In the above equation, n defines the buckling mode and I is the structure's second moment of area. As a hollow cylinder is the most similar classical structure to the studied carbon nanotubes, Eq. (3) defined for a hollow cylinder is used for obtaining the analytical results.

$$I = \pi [(d+t)^4 - (d-t)^4]/64, \tag{3}$$

in which t is the thickness of the tube's shell which is considered to be equal to 0.34 nm [4, 5, 7] in case of single-walled carbon nanotubes and d is the diameter of the pertaining tube.

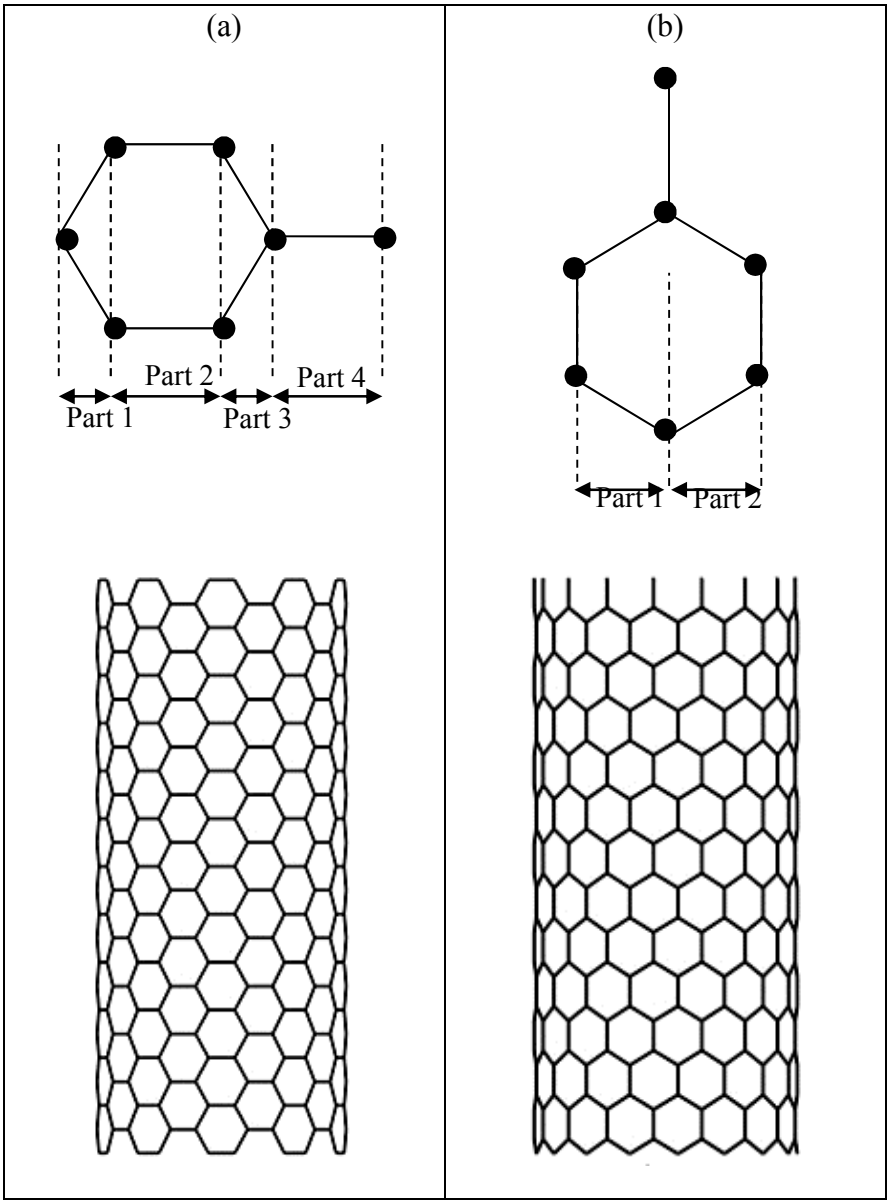

Figure 2. Front view of the unit cell and whole tube of (a) armchair, and (b) zigzag SWCNT.

As mentioned above, the applied boundary condition plays an important role in the reaction of the studied structure under load. This influence is described by the concept of the *effective length* for a classic column structure that is presented as parameter K in Eq. (2).

There are four different classical modes for buckling and four pertaining effective length parameters for each. The theoretical K values are defined for a column structure. These different modes of boundary condition and different possible buckling behaviours are shown schematically in Figure 3. The appropriate theoretical value of K is given for each case.

On the other hand, the natural or resonance frequency of a structure depends on its geometry and mass as well as the applied boundary conditions. For a beam element, under the cantilever boundary conditions, the first mode of resonance frequency in Hz, can be calculated by the following equation:

$$f_1 = \frac{1}{2\pi}\, 3.5156 \sqrt{\frac{E\,I}{\bar{m}\,L^4}}, \qquad (4)$$

in which $\bar{m}$ is the structure's mass density, i.e. mass per unit length, E is the structure's axial Young's modulus, L is the length of the tube and I is the model's second moment of area. Second and third modes of frequency are equal to f_2= 6.268 f_1 and f_3= 17.456 f_1, respectively [9, 13].

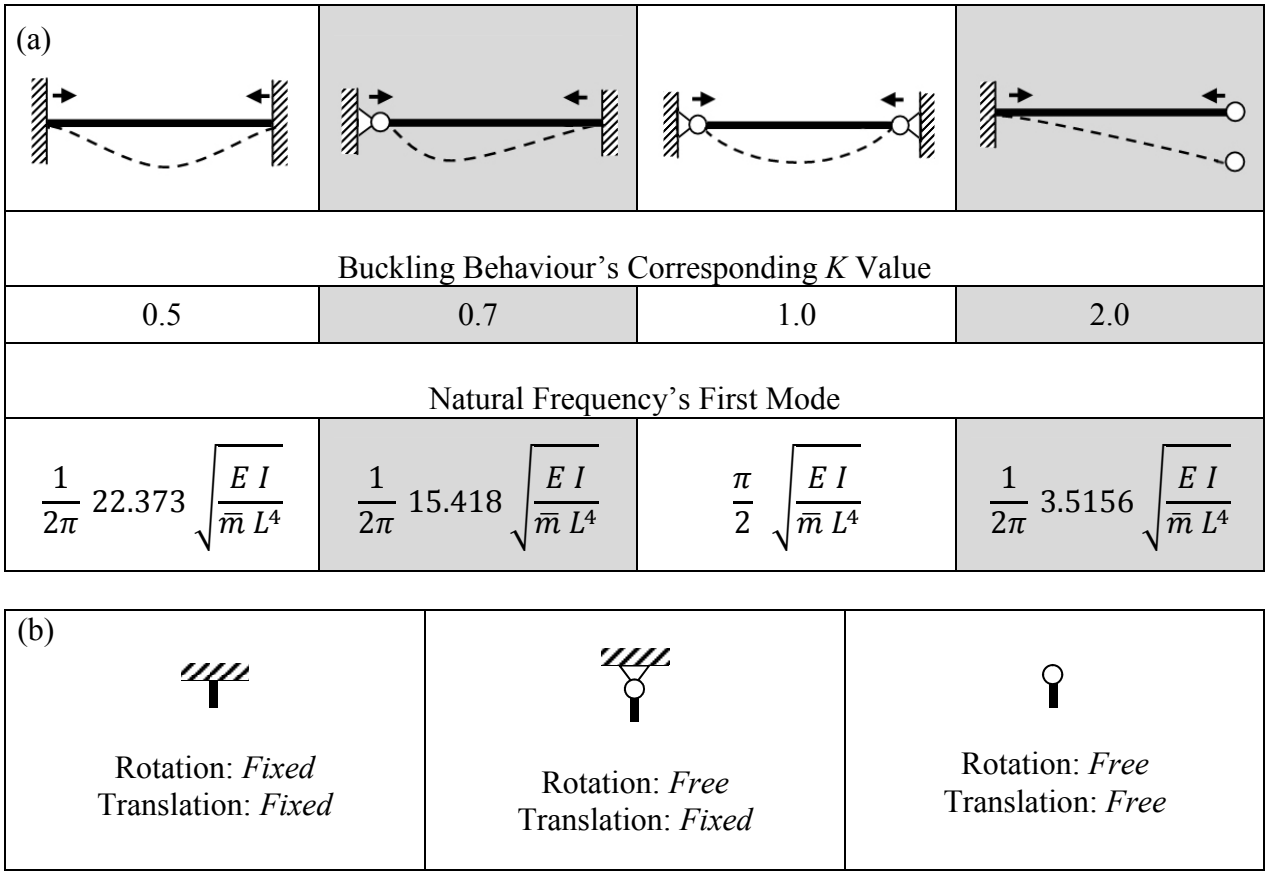

Figure 3. (a) Classical boundary conditions and their corresponding effective length constants for buckling and their first resonance frequency equation, (b) definitions of the symbols of applied boundary conditions.

Results

Buckling Behaviour. Let us consider the boundary condition of the carbon nanotubes as fixed from moving and rotating on one end and free to move on the other. As explained before, this boundary condition is known as the *Cantilever* boundary condition and the corresponding K value for this case is (K = 2).

Based on above basic definitions, the critical buckling load for both armchair and zigzag structures were modelled by the finite element software MSC.Marc and furthermore it was calculated analytically using Eq. (2). Table 1 shows the accuracy of the obtained values.

Table 1. Comparing the analytical solution of zigzag and armchair SWCNTs critical buckling load, with the optimized finite element results.

Carbon nanotube type	Analytical solution (nN)	Finite element result (nN)	Error
(10, 10) Armchair SWCNT	3.668	3.664	0.10%
(17, 0) Zigzag SWCNT	3.447	3.446	0.03%

Figure 4 represents the initial buckling behaviour of zigzag and armchair SWCNTs.

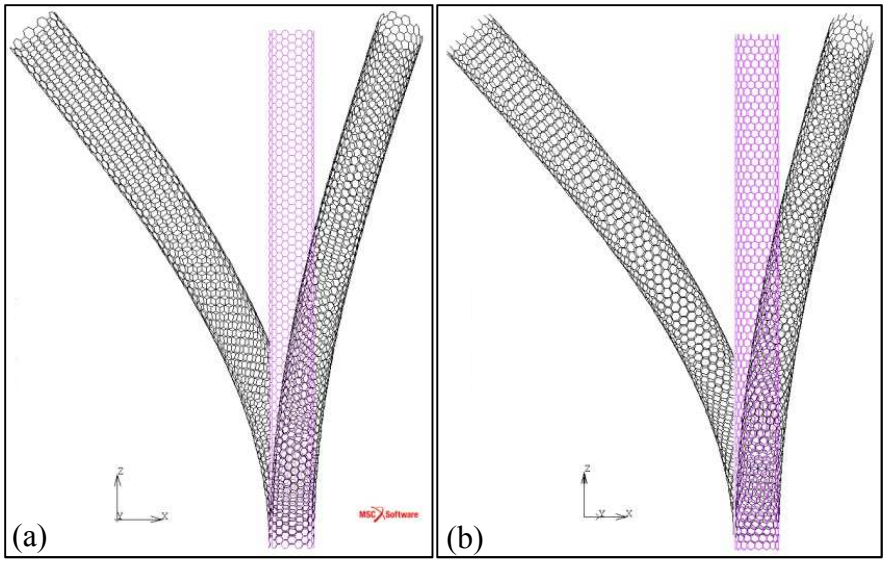

Figure 4. Buckling behaviour of (a) (10, 10) armchair and (b) (17, 0) zigzag SWCNTs.

In order to study the effect of meshing on the obtained results, the structure of (10, 10) armchair SWCNT was divided into an almost five times finer mesh. The results show the difference between the obtained results for the model with 2580 nodes and the model with 14130 nodes is absolutely negligible. As the difference of the results was about 0.03%, the model with fewer nodes was taken into consideration; as the more number of nodes are, the more evaluation time is required in each evaluation.

Resonance Frequency. The same procedure was taken in order to obtain the most accurate finite element results for the structure's natural frequency, compared to the analytical solution for armchair and zigzag single-walled carbon nanotubes.

Like the previous case, the single-walled carbon nanotubes were restricted under a cantilever type boundary condition. By defining the appropriate mass density in the finite element program, the structures' first two modes of natural frequency were simulated and compared with the calculated analytical results. Table 2 shows the obtained results for the first and the second frequency modes. As can be observed, the finite element results are in good agreement with the analytical solution of the problem solved for a hollow cylinder.

Table 2. Comparing the analytical solution of zigzag and armchair SWCNTs resonance frequency, with the optimized finite element results.

Carbon nanotube type	Results	Frequency mode1 (GHz)	Frequency mode2 (GHz)
(10, 10) Armchair SWCNT	Analytical	23.97	150.2
	Finite Element	23.94	141.1
	Error	0.12%	6.05%
(17, 0) Zigzag SWCNT	Analytical	23.44	146.9
	Finite Element	23.43	138.6
	Error	0.04%	5.65%

Figure 5 shows the different modes of deviation of a (17, 0) single-walled carbon nanotube around its initial straight mode.

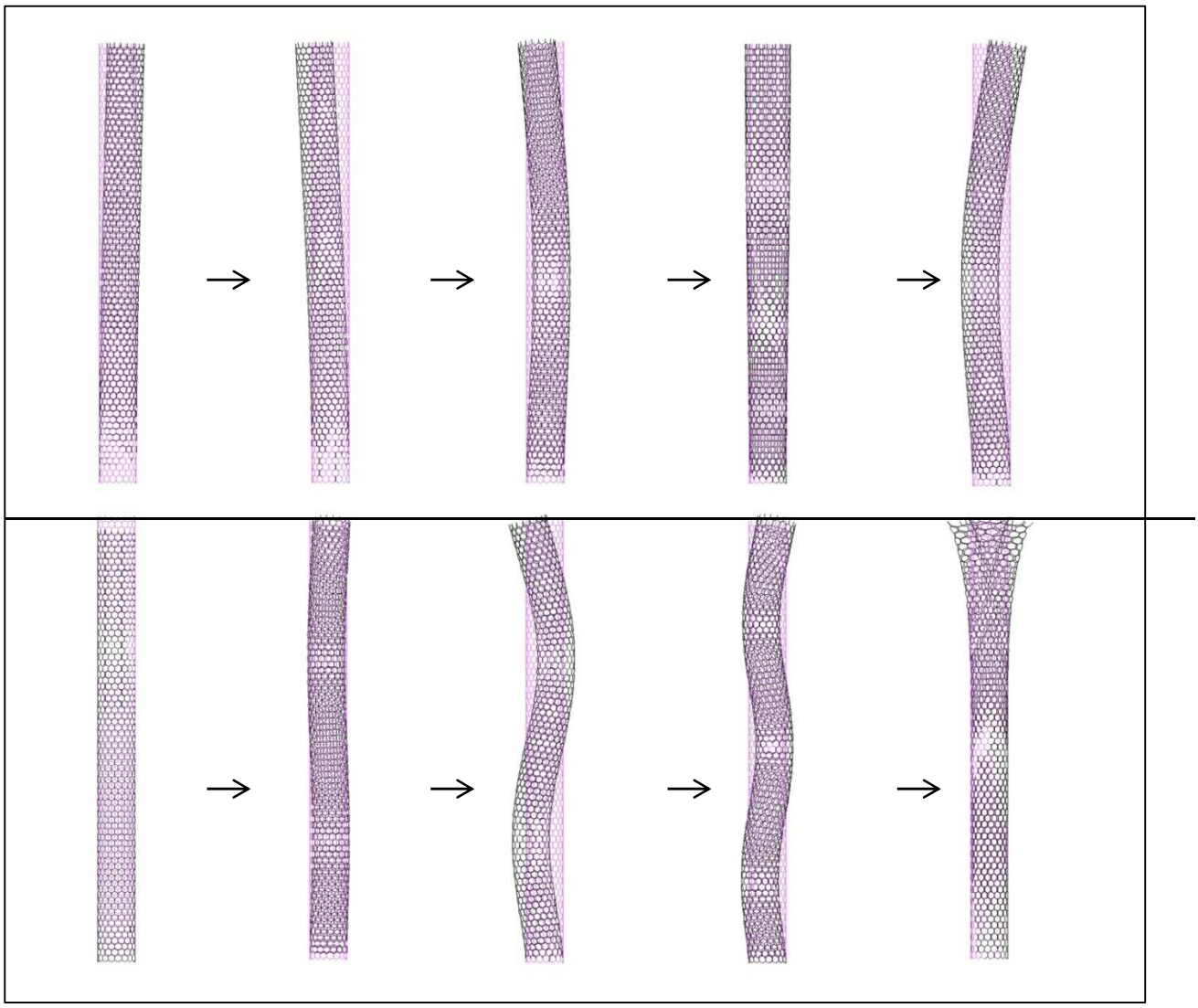

Figure 5. Frequency modes of a (17, 0) zigzag SWCNTs under cantilever boundary condition.

Conclusion

According to our investigations, the behaviour of single-walled carbon nanotubes under cantilever boundary conditions follows the prediction of the classical Euler equation. Better and more accurate results are obtained if the amount of applied load in the finite element modelling is optimized for both zigzag and armchair structures.

Toward achieving the most accurate results with comparison to the analytical solution for a hollow cylinder, a finer mesh of the armchair carbon nanotube was tested under similar conditions. Results confirm that refining the mesh does not have a significant influence on the obtained critical load of the studied SWCNT.

There was a very good agreement between the analytical and FEM results of the studied SWCNTs, however obtained finite element results, in higher modes of frequency, is not as accurate as the achieved value of the first mode.

References

1. M.S. Dresselhaus, G. Dresselhaus, R. Saito, Physics of Carbon Nanotubes, Carbon 33 (7) (1995) 883–91
2. E.T. Thostenson, Z. Ren, T.W. Chou, Advances in the Science and Technology of Carbon Nanotubes and Their Composites: A Review, Compos. Sci. Technol. 61 (2001) 1899–1912
3. M. Rahmandoust and A. Öchsner, Influence of Structural Imperfections and Doping on the Mechanical Properties of Single-walled Carbon Nanotubes, J. Nano Res. 6 (2009) 185–196
4. M. Rahmandoust and A. Öchsner, On Finite Element Modeling of Single and Multi-walled Carbon Nanotubes. J. Nanosci. Nanotech. 12 (2012) in press
5. C. Li, T.W. Chou, A Structural Mechanics Approach for the Analysis of Carbon Nanotubes, Int. J. Solids Struct. 40 (2003) 2487–2499
6. C.M. Wang, Y.Y. Zhang, Y. Xiang, and J.N. Reddy, Recent Studies on Buckling of Carbon Nanotubes, Appl. Mech. Rev. 63 (2010) 030804–1–18
7. W.S. To Cho, Bending and Shear Moduli of Single-walled Carbon Nanotubes, Finite Elem. Anal. Des. 42 (2006) 404–413
8. S.M. Mavalizadeh, M. Rahmandoust and A. Öchsner, Numerical Investigation of the Overall Stiffness of Carbon Nanotubebased Composite Materials, J. Nano Res. 13 (2011) 47–59
9. C.W. Fan, Y.Y. Liu and C. Hwu, Finite Element Simulation for Estimating the Mechanical Properties of Multi-walled Carbon Nanotubes, Appl. Phys. A 95 (2009) 819–831
10. I. Eslami Afrooz, A. Öchsner and M. Rahmandoust, Effects of the carbon nanotube distribution on the macroscopic stiffness of composite materials, Comp. Mater. Sci. 51 (2012) 422–429
11. H.J. De Los Santos, Introduction to Microelectromechanical Microwave Systems, Artech House Publishers, London (1999)
12. P.J.F. Harris, Carbon Nanotubes Composites. Maney for the institute of materials, minerals and mining and ASM international, Int. Mater. Rev. 49 (2004) 31–43
13. T. Irvine, Application of the Newton-Raphson Method to Vibration Problems, Vibrationdata Publications, 1999