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Buckling Analysis of Single Walled Carbon Nanotubes under Torsional and Axial Combined Loading by Finite Element Method

Mohsen asadipour[1], Sima Ziaee[2], Abbas Niknejad[3]

[1]Msc of Mechanics., National Iranian Oil Company
[2,3]Assistant Prof., Yasouj University, Mechanical Department
Corresponding author: Mohsen Asadipour

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ABSTRACT

In This paper, Buckling phenomenon of single walled carbon nanotubes under torsional and axial combined loading by finite element method is investigated. Models are constructed via an individual structural model in Ansys software. CNTs hexagon geometrical structure is simulated by means of porous shell. Single walled carbon nanotubes of zigzag (12,0) and (21,0)with various aspect ratios (length to diameter ratio) are selected and they are subjected to torsional and axial combined loads. In this study, the effects of radius, length and aspect ratio on the critical buckling loads are investigated. Numerical results indicate that with increment of length and aspect ratio, the critical buckling loads will decrease generally. Also diagrams show that In lengths greater than 5 nm, nanotubes (21,0) will endure more critical buckling loads relative to nanotube (12,0). This result is followed by the increase in surface area by increasing the diameter of the nanotube. In this study the changes trend of critical buckling loads In terms of the different variables is good agreement with previous studies.

KEYWORDS: Finite element; Porousshell; Zigzag nanotube; Aspect ratios; combined loading.

1 INTRODUCTION

Since the discovery of carbon nanotubes (CNTs) by Sumio Iijima (Iijima,1991), they have played an essential role in leading the extensive progress of Nano scale science and technology during the past two decades. These small structures are found to be possessing extraordinary mechanical, thermal and electrical properties compared to conventional structures. Due to these superior properties, CNTs are used in the emerging fields of Nano electronics and Nano devices. Beside due to the rewardable physical and mechanical properties such as high stiffness to weight ratio, high strength and resilience, superb thermal and electrical conductivities of carbon nanotubes, a strong motivation has been generated to investigate the CNT-related fields (Treacy et al, 1996; Lu, 1997; Lourie et al, 1998; Zhou et al, 2000; Ru, 2000; Kudin et al, 2001; Tu et al, 2002; Jin et al, 2003; Pantano et al, 2004; Chang et al, 2005).Generally there are primarily three modeling methods for the buckling analysis of CNTs, namely, experiments, atomistic simulations, and continuum mechanics models. Experiments at Nano scale are themselves still under development and thus have resulted in a range of values for various mechanical properties. The experiments at this Nano size are difficult to be controlled accurately. Accordingly, the theoretical analyses of Nano structures are becoming increasingly important. Atomistic simulations can accurately map out the structure of CNTs and effectively simulate the deformation of CNTs under various conditions. However, due to whopping computational expense, atomistic simulations are currently limited to small length and small time scales, which lead to the effort for other more efficient ways to investigate the buckling stability of CNTs, such a continuum mechanics theory. Ordinarily, there are four research methods based on continuum mechanics theory, including the elastic beam model (Govindjee et al, 1999; Harik, 2000), the elastic cylindrical shell model (Ru, 2000; He et al, 2005),the molecular structure mechanics and the finite element method (FEM). Yakobson et al. introduced an atomistic model for buckling of SWCNTs and also compared it with a simple continuum shell model (Yakobson et al, 1996). They found that the continuum shell model could predict all changes of buckling patterns in the MD simulations. As an alternative, the simple continuum shell model is used to investigate buckling behavior of CNTs (Ru, 2001; Arroyo et al, 2003; Han et al, 2003; Xiao et al, 2004; Han et al, 2005; Cao et al, 2006; Yao et al, 2007). Although continuum theories that are directly linked to atomistic models seem to provide reliable results, the formulation of the methods is still quite complicated and usually much more computationally expensive than a finite element approach based on conventional elasticity theories. The FEM is rather mature and now it has been regarded as the most powerful tool for computer analysis and simulations. Recently great efforts have been made to extend FEM for the analysis of CNTs (Pantano, 2003; Wang, 2006).As we all known the initial geometric imperfection has a significant effect on

*** Corresponding Author:** Mohsen Asadipour, Msc of Mechanics., National Iranian Oil Company

the buckling and post buckling behavior of carbon nanotubes (Zhou, 1994; Ding, 2005). Meo and Rossi, 2006 to develop a finite element model based on molecular mechanics to predict the ultimate strength and strain of single walled carbon nanotubes (SWCNT). The interactions between atoms were modeled by combining the use of non-linear elastic and torsional elastic spring. This study is done on the zigzag, armchair and chiralnano tubes under non-axial loads (Meo and Rossi, 2006).Wang et al, 2009 designed the twist of carbon nanotubes using atomic molecular dynamic simulations. The ultimate twist angle per unit length and the deformation energy are calculated for nanotubes of different geometries. It is found that the big tube is harder to be twisted while the small tube exhibits higher ultimate twisting ratio. For multi-walled nanotubes, the zigzag tube is found to be able to stand more deformation than the armchair one. They observed the surface transformation during twisting. Formation of structural defects is observed prior to fracture (Wang et al, 2009). In 2012 year, Lashkari Zadeh et al investigated buckling behavior of perfect and defective DWCNTs under axial, bending and torsional loadings via a structural mechanics approach. They found that vacancy defects greatly reduce the critical buckling load of DWCNTs and the density of defects plays an important role in buckling of DWCNTs (Lashkari Zadeh et al, 2012).

2 Analysis method and design of models

2.1 Buckling analysis method

Due to difficulties of analysis of carbon nanotubes by means of classical or analytical methods, the utilization of numerical methods such as finite element is very benefit. Accordingly, investigation and analysis of shells, particular cylindrical shells by finite element method are considered in the last years. In this method shell surface is divided to very gracile elements that are connected together at nodes when as forces and nodal displacements are appertained together with stiffness matrix parameter $[k_e]$. In this section, finite element stiffness matrix of shell buckling analysis is obtained by element strain energy relation that can be shown as:

$$\frac{1}{2}\delta^2 V = \frac{1}{2}\int_{S_1}^{S_2}(\{\varepsilon\}^T[C]\{\varepsilon\} + \lambda\{\beta\}^T[N_0]\{\beta\})rds \quad (1)$$

Where $\{\varepsilon\}$ and $\{\beta\}$ denotes the strain and rotation vectors, $[c]$ and $[N_0]$ delineates fundamental equations coefficients and membrane forces respectively. By considering strain and rotation vectors unit age displacements, integration on shell element from s_1 to s_2 and by use of Gaussian integral, equation (1) is defined as:

$$\delta^2 V^e = \{u\}^T([K]^e + \lambda[N]^e)\{u\} \quad (2)$$

Where $[K]^e$ is element stiffness matrix and $[N]^e$ is geometric stiffness matrix. Energy is released suddenly while buckling phenomenon occurs. i.e.,

$$([K] + \lambda[N])\{u\} = 0 \quad (3)$$

The above equation is established while:

$$|[K] + \lambda[N]| = 0 \quad (4)$$

Finally by solving relation (4), the load critical parameter (λ) and there in after buckling critical load can be obtained. This approach to determining the critical buckling load is known as the bifurcation or eigenvalue method.

2.2 Design of models

In this work, carbon nanotubes hexagon geometrical lattice is simulated by means of porous shell. In fact C-C synthesis of carbon nanotubes ($a_{c\text{-}c}$= 0.142 nm) are constructed by cut out of hexagonal cell on the continuum cylindrical shell (see Figure 1). So (12,0) and (21,0) zigzag carbon nanotubes with various aspect ratios (length to diameter ratio) are modeled(see Table 1 and 2). In the modeling procedure, the eight-node shell 93 element has been used to extract the FE simulation for carbon nanotubes. Beside constructed models include young's modulus E=5.5 Tpa, Poisson's ratio ν=0.3 and effective wall thickness t=0.066nm, respectively (Yakobson et al, 1996).

Table 1.Lengths and aspects ratio of SWCNTs for zigzag (12,0)

Length (nm)	1.56	3.27	4.97	6.67	8.38	10.08	11.78
(L/D)	1.64	3.44	5.23	7.02	8.82	10.61	12.40

Table 2.Lengths and aspects ratio of SWCNTs for zigzag (21,0)

Length (nm)	1.56	3.27	4.97	6.67	8.38	10.08	11.78
(*L/D*)	0.95	2	3.03	4.06	5.10	6.14	7.18

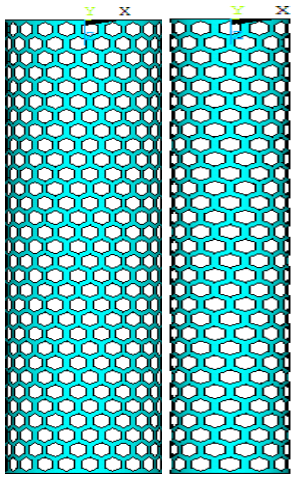


Figure 1.Schematics of SWCNTs (12,0) and (21,0)

3 RESULTS AND DISCUSSION

Based on the analysis procedure in this paper, the torsional and axial loads are distributed on one end of the nanotube simultaneously, while the other end of the nanotube is assumed to be fixed. Also the load aspect λ=1 is considered. Then the effects of length (*L*) and especially nanotube aspect ratio (*L/D*) on the buckling forces have been discerned. In figure 2 the cross-sectional views of the nanotubes after buckling process is shown in three different modes. In this figure both axial and torsional loads caused by the deformation of the nanotube cross section is visible.

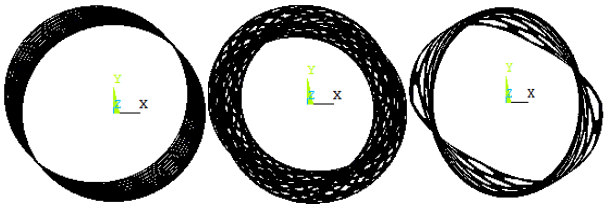
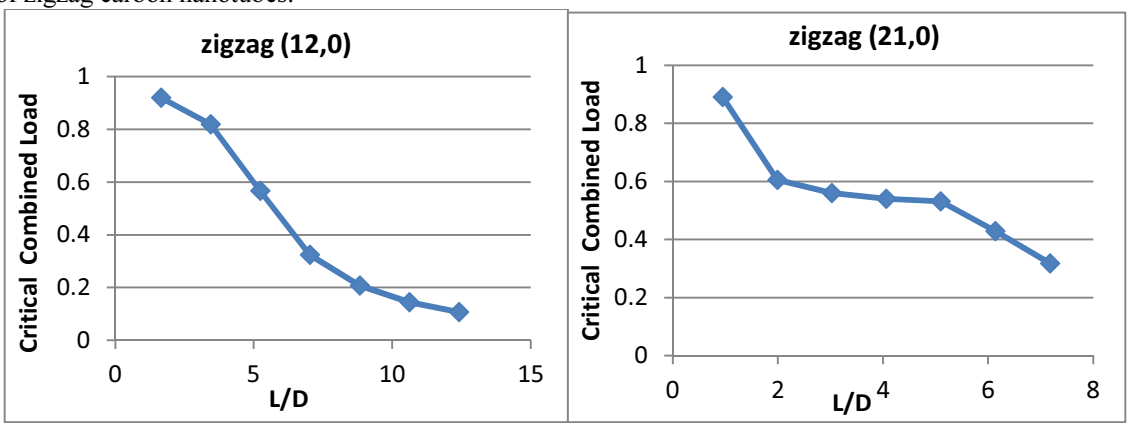


Figure 2.Views of the nanotube cross-section after buckling in three different modes

The critical combined buckling loads for (12,0) and (21,0) zigzag carbon nanotubes with various aspect ratios are executed in figure3. Diagrams show that with the increase of the aspect ratio, critical buckling loads reduce for both of zigzag carbon nanotubes.



(a) (b)

Figure 3.Critical combined loads versus various aspect ratio for (a) zigzag (12,0) and (b) zigzag (21,0)

In figure 4 the critical combined buckling loads in terms of nanotube length for (12,0) and (21,0) zigzag carbon nanotubes are displayed. By comparing the curves in this figure, it is observed that In lengths greater than5 nm, nanotubes (21,0) will endure more critical buckling loads relative to nanotube (12,0). This result is followed by the increase in surface area by increasing the diameter of the nanotube. Also it is apperceived that the decrease trend of critical buckling loads In terms of nanotube length is similar than the decrease trend of critical buckling loads In terms of nanotube aspect ratio.

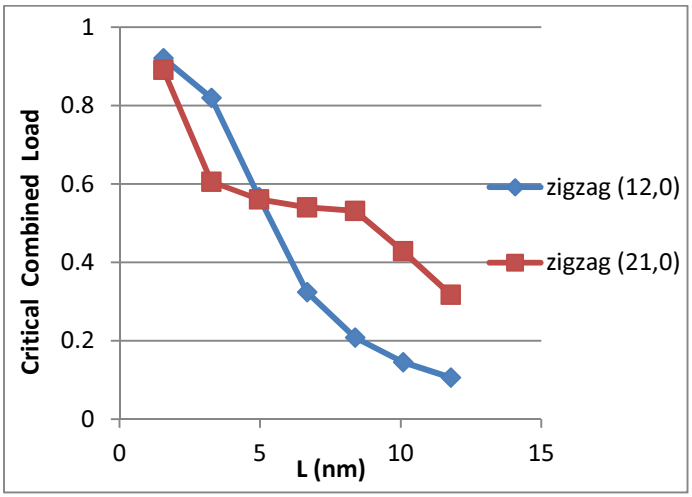


Figure 4.Critical combined loads versus various length for zigzag (12,0) and zigzag (21,0)

4 Conclusions

In This article, buckling phenomenon analysis of single walled carbon nanotubes under torsional and axial combined loading by finite element method is done. Single walled carbon nanotubes of zigzag (12,0) and (21,0) with various length and aspect ratios (length to diameter ratio) are selected and are simulated based on FEM (Ansys software) by an individual structural model that it is named a porous shell. The computational results have led to the following conclusions:

1. Length, diameter and length to diameter ratio (L/D) are significant parameters in buckling analysis of SWCNTs under torsional and axial combined loading.
2. With increasing aspect ratio and the length of the nanotube, critical torsional and axial combined loads reduced.
3. In a similar length (Lengths greater than 5 nm) Nanotubes with a diameter larger endure more critical combined loads Due to the increased surface area and increase its strength.

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