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Continuum modeling based buckling analysis of Single walled Nanotube

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***Abstract*—This paper represents the buckling behavior of different atomic structures of single walled nanotubes. The buckling behavior is important to analyze, to understand how the nanotube will behave in applications, where they are subjected to compressive loading. The single walled carbon nanotubes (CNTs) and boron nitride nanotubes (BNNTs) have been considered for the analysis to analyze the buckling behavior in terms of critical buckling force and buckling strain under compressive forces. In the present work, continuum solid modeling based analytical approach has been consider to analyze the critical buckling force for different nanotube materials; CNT and BNNT, as well as for different atomic structures of the nanotubes armchair (3,3) and zigzag (5,0). The single walled nanotube are modelled as continuum hollow tube with effective thickness, which is an approximation of the real atomistic structure of the nanotubes. The analysis has been performed to analyze the effect of variation in length in terms of aspect ratio (length/diameter) and variation in diameter of the nanotube. From the analysis it is found that BNNTs are having higher values of critical buckling force compare to CNTs for both types of considered atomic structures of the nanotube. Also, it is found that as the length increases the value of critical buckling load decreases irrespective of material and types of atomic structure.**

Keywords: Critical buckling load, Buckling strain, CNT, BNNT

I. INTRODUCTION

Carbon nanotubes (CNTs) have been subjected to intensive Study since their discovery in 1991 due to their unique Combinations of mechanical, electrical and chemical Properties.[1–5].In order to fulfill their promising applications Such as Nano strain sensors and actuators, Nano fluidic components, and carbon nanotube-reinforced composites, the mechanical properties of CNTs must be fully understood. AVariety of experimental works have been put together to investigate the elastic properties of CNTs, focusing on Young's moduli. Tracey and co-workers have pioneered the measurement of thermally induced vibration amplitudes of CNT cantilevers from 20 to 800 °C: for multi-walled carbon nanotubes (MWCNTs) and single-walled carbon nanotubes (SWCNTs), the effective Young's moduli of reported to be in The ranges of 0.40–4.15 TPa and 0.9–1.9 TPa respectively. Alternatively, by using an atomic force microscope (AFM) tip to bend a MWCNT cantilever, the Young's moduli of MWCNTs are found to be 1.28±0.59 TPa. Besides the studies of CNT elastic properties at small deformation, the mechanical response of CNTs under large deformation has begun to receive wide attention: in particular, the buckling behaviors of CNTs subjecting to excess deformation have been observed.[1,9,10]Experimental investigations have also shown that the buckling deformation of CNTs under very large strain can be completely recovered after unloading.[9,11,12]It is found that the physical properties such as conductance of CNTs are strongly influenced by the occurrence of buckling.[13]Thus, the reversible transformation Between the buckled state and normal state of CNTs may Lead to potential applications such as Nano electronic devices(Nano-transistors), [13]Nano-fluid components (Nano-valve) [14]And reversible elements in Nanoelectromechanical systems .In view of both mechanical integrity and application, it is Very important to understand the buckling mechanisms of CNTs . And a boron nitride nanotube (BNNT) can also be imagined as a rolled up hexagonal BN layers or as a carbon nanotube (CNT) [15,16]in Which alternating B and N atoms entirely substitute for C atoms .Similar to CNTs, BNNTs have chirality's, an important geometrical Parameter. BNNTs, which possess a similar morphology as CNTs but distinct properties of their own, appear to be potential Candidates for biomedical applications due to their uniformity and stability in dispersion in solution [17].Unlike CNTs, whose Electronic structure and properties vary widely based upon tube helicity, concentric layers, and soforth, the BNNTs are semiconducting regardless of their diameter and chirality's[18]. The experimental investigation of buckling behavior remains a challenge because of difficulties encountered at the Nano-scale.[9] And, The main objective of this paper is to evaluate effects of nanotube diameter, length, and tube chirality on the buckling force and buckling strains of nanotubes which could be helpful to get the insights of buckling behavior of nanotubes

II. COMPUTATIONAL METHOD

The computational approach is better by providing simulation results to help the understanding, analysis and design of such Nanotube. There were two theoretical and numerical approaches: molecular dynamics and continuum mechanics.

From the viewpoint of molecular mechanics, a nanotube can be regarded as a large molecule consisting of carbon or boron atoms. The atomic nuclei can be regarded as material points. Their motions are regulated by a force field, which is generated by electron–nucleus interactions and nucleus–nucleus interactions Machida, 1999 [19]. Usually, the force field is expressed in the form of steric potential energy. It depends solely on the relative positions of the nuclei constituting the molecule. And by Continuum Mechanics meaning Nanotubes can be primarily modeled as continuous beams or thin shells with a fixed effective wall thickness, young's modulus and Poisson's ratio. The main objective of this paper is to evaluate the buckling force of nanotubes which could be helpful to get the insights of buckling behavior of nanotubes. In particular, tube chirality is known to have a strong influence on the electronic properties of carbon nanotubes. Graphite is considered to be a semi-metal, but it has been shown that nanotubes can be either metallic or semi-conducting, depending on tube chirality (Dresselhaus et al., 1996) [22].

Based on the modeling procedure described above, buckling behaviors have been studied for Nanotubes under compression.

If the nanotube is assumed as a continuum Cylindrical shell with appropriate wall thickness Dresselhaus et al., 1995[22], the critical loading can be calculated according to the classical Euler formula for cantilever columns Chen and Lui, 1987[23]

Here, K =Effective length of column,

=Critical compressive force(nN)

(1)

For rods/tubes with pinned ends, k=1
For rods/tubes with clamped ends, k=4
For rods/tubes with clamped-free ends=2

Whereas, $$I = \frac{\pi}{64}({d_o}^4 - {d_i}^4) \qquad (2)$$

Here, $d_o = outer\ daiameter\ of\ nanorods/$
$d_i = outer\ daiameter\ of\ nanorods/tubes$

Where E is the Young's modulus of the carbon Nanotube in (TPA), I is the cross-sectional Inertia about one of its symmetric axes and l is the nanotube length.

III. CONTINUUM SHELL MODELLING

The buckling behaviors of NTs under axial compression have been investigated by using the continuum shell model and beam model. [15, 17] When the aspect ratio of NT, which is defined as the ratio between the tubes Length, *l*, and the tube diameter, *d*, is larger than 50, the Mechanical behavior of NTs approaches that of a beam. In the present work NT at macro level is modeled as a tubular structure in consideration with effective constants such as elastic modulus, shell or wall thickness which are of CM meaning. Yakobsonet.al [20**]** and Pantano et.al **[**[21]

IV. NANOTUBE UNDER COMPRESSION

In order to reveal the effect of the chirality on the axial compression of the NTs, several tubes with Different chirality's and lengths are selected. These chirality's include (3,3),(5,0)and (8,8),(10,10),(12,12),(15,15), (17,17),(20,20) and (23,23) for SWCNT and SWBNNT . To include the effect of diameter, and constant aspect ratio the set of tubes with said chirality's above, are also investigated. In addition, the diameters of these tubes are varied.

V. RESULTS AND DISCUSSION

For the present work the continuum model for CNT and BNNT is approximated by considering thickness of 0.066nm [19] and 0.065nm [25] for latter. Elastic modulus for BNNT was found to be as 1.24TPa and for CNT 1TPa. The analytical results were being explained over here for the nanotube under compression and critical compressive force were evaluated from equation (1) as mentioned above. The effective length of the nanotube was taken as 4 when one end is fixed and other end is free. The evaluation of the critical compressive force was done for armchair and zigzag configuration. For armchair (3, 3) CNT diameter was found to be 0.4071nm and for armchair (3, 3) BNNT was 0.4211nm.And, from atomistic point of view Bond lengths were reported to be 0.1421nm for CNT and0.147nm of BNNT.

The results were computed analytically which could be useful for the analysis of NTs on macroscopic level for the said configuration and parameters to get the insights of buckling.

The Table I and Table II. Represents the results of the nanotube length for increasing nanotube aspect ratio for critical compressive force and consecutively values for the other configurations were computed.

TABLE I. ELASTIC PARAMETERS

Sr no.	**Armchair(3,3)CNT**		
	(l/d)	*l(nm)*	$F_{cr}(nN)$
1	2	0.8142	3.9657784
2	4	0.16284	0.991446
3	6	0.24426	0.440642
4	8	0.32568	0.2478611
5	10	0.4071	0.1586311

TABLE II. ELASTIC PARAMETERS

Sr no.	**Armchair(3,3)BNNT**		
	(l/d)	*l(nm)*	$F_{cr}(nN)$
1	2	0.8422	5.1929179
2	4	0.16844	1.28243
3	6	0.25266	0.569969
4	8	0.33688	0.320607
5	10	0.4211	0.205189

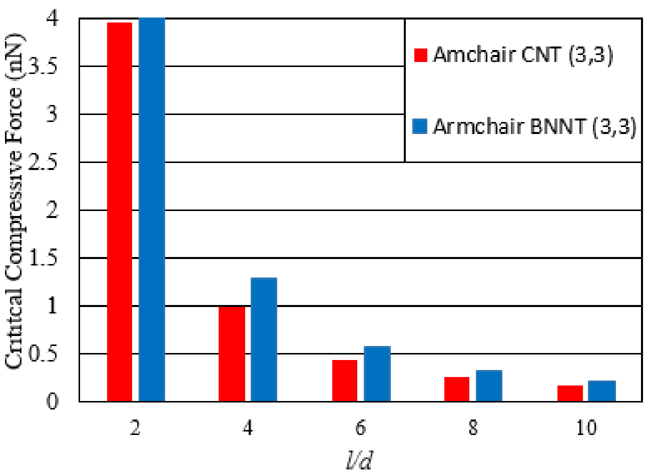


Fig1.Comparison of armchair (3, 3) CNT and BNNT for the effect of nanotube aspect ratio on critical compressive buckling force

Here, Fig1. Shows the buckling force which is varying with the Nanotube aspect ratio 1-2 keeping nanotube diameter constant. It is observed that with increase of nanotube aspect ratio buckling force decreases. The buckling force for Armchair CNT decreases more steeply than Armchair of BNNT. Further it's also been evaluated for Zigzag CNT and BNNT.

Table III and IV represents the elastic parameters of zigzag (5,0) CNT and zigzag(5,0)BNNT for the parametric variations.

TABLE III. ELASTIC PARAMETERS

Sr no.	**Zigzag(5,0)CNT**		
	(l/d)	*l(nm)*	$F_{cr}(nN)$
1	2	0.7834	3.7423648
2	4	0.15668	0.9355912
3	6	0.23502	0.4158183
4	8	0.31336	0.2338978
5	10	0.3917	0.1496946

TABLE IV. ELASTIC PARAMETERS

Sr no.	**Zigzag(5,0)BNNT**		
	(l/d)	*l(nm)*	$F_{cr}(nN)$
1	2	0.081	4.846
2	4	0.162	1.211
3	6	0.244	0.775
4	8	0.324	0.538
5	10	0.406	0.194

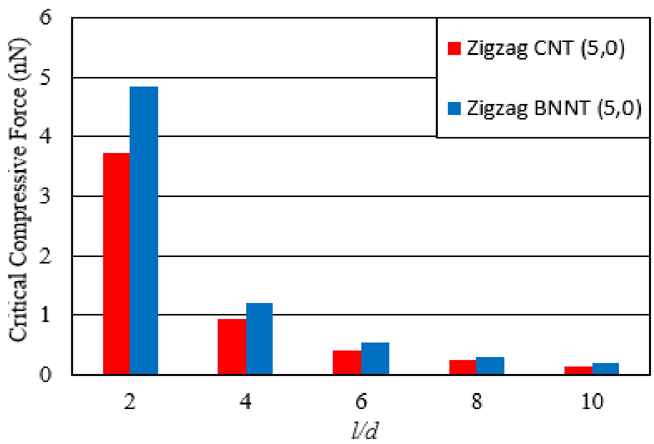


Fig2. Comparison of zigzag (5, 0) CNT and BNNT for the effect of nanotube aspect ratio on critical compressive buckling force

This Fig2.depictsthe comparison for very small length of aspect ratio1-2. It was observed that critical buckling force decrease more steeply for zigzag CNT than BNNT. Fig3 and Fig4. Represents the buckling force results of nanotubes with when diameter is varying. And Aspect ratio is kept constant

Furthermore, the diameter variations for the said configurations has been done and their respective critical force values are mentioned in following Table V and Tale VI

TABLE V. EFFECT OF VARIATION IN DIAMETER ON CRITICAL COMPRESSIVE FORCE FOR ARMCHAIR CNT

Sr no.	Armchair (3,3) CNT	
	do(nm)	$F_{cr}(nN)$
1	0.268	0.966
2	0.46	1.714
3	0.668	2.486
4	0.868	3.268
5	0.107	4.055

TABLE VI. EFFECT OF VARIATION IN DIAMETER ON CRITICAL COMPRESSIVE FORCE FOR ARMCHAIR BNNT

Sr no.	Armchair (3,3) BNNT	
	do(nm)	$F_{cr}(nN)$
1	0.270	1.188279
2	0.470	2.10366
3	0.670	3.047329
4	0.870	4.002973
5	0.107	4.964793

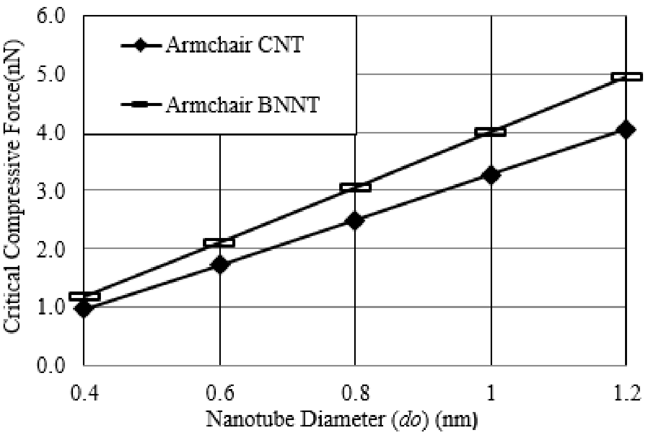
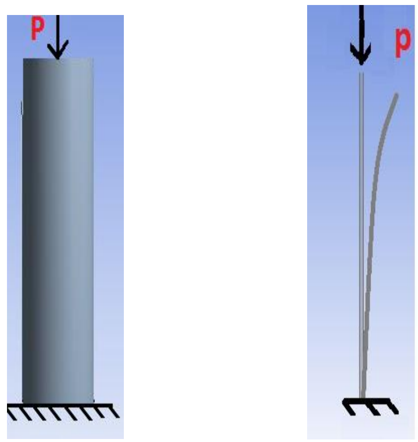


Fig3. Comparison of armchair (3, 3) CNT and BNNT for the effect of nanotube diameter on critical compressive buckling force.

Figure 3 represents the buckling force results of nanotubes when nanotube diameter is varying. Starting From the small range of 0.4-0.6, the critical buckling force was found to have increasing trend. CNTs were found to have higher values than BNNTs.

VI. SIMULATION APPROACH

The approach used over here for simulation was Eigen value buckling analysis and was carried out in Ansys17.1.
The model which was generated in modelling software with appropriate geometrical parameters was imported to the analysis software. And the boundary condition chosen for the same is shown below.



(a) (b)

Fig4. Illustration of (a) a tubular model and (b) deformation mode corresponding to axial compression

The analytical and simulation results for CNTs were reported to have higher buckling force for BNNTs. And Moreover The percentage difference was reported to be 29.34Of CNT and of BNNT was 29.48.
As far as the buckling is concerned it is a deformation process in which a strain beyond a threshold causes an abrupt change in the deformation profile. So, to have the idea about the buckling behavior. The configurations in above sections mentioned were investigated by numerical analysis and simulations too.
As the critical compressive buckling strain decreases rapidly for NTs having small aspect ratio, their mechanical behaviors are found to be close to that of thin shells.
The buckling strains of Single Walled Carbon Nanotube and Single Walled boron nitride Nanotube were compared with respect to the nanotube diameter variations because of the elastic properties and mechanical responses that has begun to attend a wide attention particularly for buckling behavior.

$$\epsilon_{cr-comp} = \frac{2}{\sqrt{3(1-\nu^2)}} \quad (3)$$

Table VII and Table VIII represents analytical and simulated critical buckling strains for the mentioned boundary condition above.

TABLE VIICRITICAL BUCKLING STRAIN VALUES FOR ARMCHAIR CNT

Sr no.	Armchair CNT			
	Chirality	*Diameter(d)*	*Analytical values*	*Simulated values*
1	(8,8)	1.09	0.0714	0.0718
2	(10,10)	1.36	0.0572	0.0605
3	(12,12)	1.63	0.0477	0.048
4	(15,15)	2.04	0.0381	0.0395
5	(17,17)	2.31	0.0336	0.0360
6	(20,20)	2.71	0.0286	0.0305
7	(23,23)	3.12	0.0249	0.0260

TABLE VIIICRITCAL BUCKLING STRAIN VALUES FOR ARMCHAIR BNNT

Sr no .	Armchair BNNT			
	Chirality	*Diameter(d)*	*Analytical values*	*Simulated values*
1	(8,8)	1.12	0.0713	0.0713
2	(10,10)	1.40	0.0571	0.0601
3	(12,12)	1.68	0.0476	0.0476
4	(15,15)	2.11	0.0381	0.0391
5	(17,17)	2.39	0.0336	0.0356
6	(20,20)	2.81	0.0285	0.0301
7	(23,23)	3.23	0.0248	0.0256

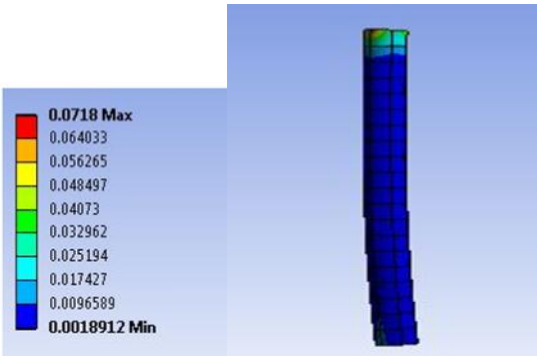


Fig 5. Comparison of armchair CNT and BNNT for the effect of critical Buckling Strain for Nanotube diameter Variations.

The Armchair CNT was found to be Have higher strain values Than BNNT for varying chirality. And the simulated values were found to be in agreement with the numerical values.

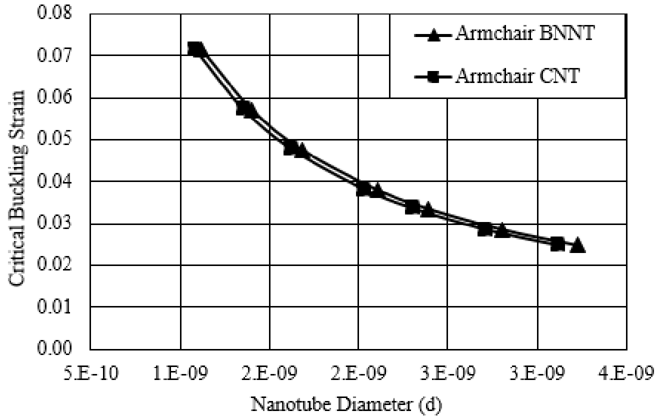


Fig 6. Comparison of armchair (3, 3) CNT and BNNT for the critical buckling strain of respective nanotube diameters

Equations used for the computation were taken from the literature [11]. The given above tables and figures below compared bending buckling curvature with respect to increasing nanotube diameter.

VII. CONCLUSIONS

- In this paper, the effects of tube chirality, elastic parameter and boundary condition on the critical compressive force of SWCNT and SWBNNT investigated because the buckling forces are sensitive to the tube chirality and end condition chosen for the analytical work.
- The influences of nanotube diameter are also included. The elastic properties are analyzed under compressions.
- Overall results indicated that when aspect ratio is increasing the critical buckling forces of CNT and BNNT was found to be decreasing but on comparison part the Zigzag turns out to have higher values than that of Armchair CNT and BNNT.
- And For constant aspect ratio and increasing nanotube diameter the critical buckling force for Zigzag was found to have increasing trend. Therefore Zigzag BNNT type of the Single Walled Nanotubes turns out to be stiffer than the Armchair type, and can be preferable for the load bearing Applications.
- Critical buckling strains were computed and reported that they are not only sensitive to the constrained boundary condition but also to the tube chirality.

- The main purpose of this paper is to provide useful insights on the effect of end condition and chirality in tube buckling.

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