

## BUCKLING BEHAVIOUR OF SINGLE WALLED SHORT CARBON NANOTUBES

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**ABSTRACT.** In the present paper the study the buckling behavior of short carbon nanotube is studied. Euler Bernoulli beam model is used for the formulation of the problem. An efficient mathematical Galerkin method with quintic splines is applied to determine the results. The impact of the size of nanotube and the effect of small scale parameter on buckling load is seen and the outputs are plotted graphically. The obtained solutions agree with those results reported in literature and determine the importance of small scale parameter in the buckling analysis of nanostructures.

2010 MATHEMATICS SUBJECT CLASSIFICATION. 70-08, 70G99.

KEYWORDS AND PHRASES. Nonlocal Elasticity Theory, Critical Buckling Load, Small Scale Effect, Carbon nanotube, Quintic splines.

### 1. INTRODUCTION

Carbon nanotube is a two dimensional hexagon lattice made up of carbon atoms. These nanotubes were first introduced by Kroto [10] in 1985 and then investigated by Iijima in 1991[31]. Starting from the invention, nanotechnology is playing its vital role in nano electromechanical machines. Due to the unique structure and possession of unique properties, the carbon nanotubes are continuously being used in several engineering applications including solar cells, micro and nano electrical and mechanical systems [40]. Mechanics of these nanostructures plays a significant role in designing the smart and efficient electromechanical systems. Therefore the analysis of mechanical behaviour of nanotubes is the key point of research for academicians as well as for researchers and continuum mechanics modeling [18] plays a central role to achieve this objective. This approach uses the basic laws such as law of energy conservation [12] or momentum. This kind of modeling needs fewer computations and thus reduces execution time. The accurate analysis of the mechanical nature helps to get the reliability and stability of these nanostructures [38]. In addition, local elasticity theory has the limitation of not capturing the size effect; therefore several generalized continuum theories are employed for further development of these nanostructures. The simulation of mechanical behavior of carbon nanotubes is performed by using several mathematical techniques [34,9]. A comparative study of the characteristics of nanobeams is done in [8]. The value of Young's modulus is predicted in [20]. Exact solutions of SWCNT have been carried out in [25,1] using different theories. Vibration response of chiral SWCNT's using Timoshenko beam model is shown in [16] and of DWCNT's has been done in [3]. Wave propagation of the carbon nanotubes is performed in [36]. A number of

exact and numerical solutions for buckling analysis of these nanostructures using various beam and shell theories are available in literature [11, 23, 26, 28, 33, 37]. Based on the chirality, the fundamental structure of SWCNTs can be described as zigzag, armchair and chiral configurations. Timoshenko (TBT) and Euler Bernoulli beam theory (EBT) is used to discuss the nature of chiral SWCNT and DWCNT in [21,15]. Several numerical techniques such as initial parameter in differential form, finite element method, differential transform method and differential quadrature methods are available in literature to study the nature of nanostructures [7,29,30,32]. Several authors in [17,19,39] applied the wavelet tool to compute the critical buckling strain/load of nanostructures. TBT theory is used to find the critical load for short carbon nanotubes in [22]. Thermal changes affect the stability of the carbon nanotubes and this study is used to capture the abrupt behavior of these small scale structures in [4]. Several beam theories are employed to analyze the nature of carbon nanotube and effect of small scale parameter is observed in [5,6,13,23,35]. Buckling is one of the reasons for loss in stability and thus causes failure of the system. Thus, the determination of buckling response of the nanostructures takes place, so that one can design the CNTs based appropriate system that can be used efficiently and accurately. In the present work, Governing system of equations is derived using Euler Bernoulli beam theory and Galerkin's approach is used to find the results. While applying Galerkin method, quintic B-splines are used as the weight function. Usage of these weight functions determines the results more accurately and their convergence is fast. Impact of length of the nanotube and of nonlocal parameter on buckling load ratio is observed and plotted graphically. Results indicate that the small scale effect plays a significant role in the buckling analysis of carbon nanotubes. Obtained results are verified with those available in literature.

## 2. FORMULATION OF THE PROBLEM

Eringen's theory states that the stress at a reference point in the system is regarded to be a function not only strain at that point but also on the strain states at all other points of the system. The nonlocal stress-strain relation using this theory can be expressed according to [2] as

$$(1) \quad (1 - \mu^2 l^2 \nabla^2) \sigma = S : \epsilon .$$

where  $\nabla^2$  is the Laplacian operator,  $L$  is the size of tube,  $\sigma$  and  $\epsilon$  are the stress and strain tensor of order two,  $S$  is elasticity tensor of order four, ':' is the double dot product and  $\mu$  is the nonlocal parameter that determines the small scale effect. It is important to note that in the absence of  $\mu$ , the nonlocal constitutive relation reduces to classical constitutive relation. EBT theory is used to formulate the equations of the problem under study. According to this theory, the equations of motion are given by

$$(2) \quad \frac{dF_A}{dx} = 0, \quad \frac{d^2 M}{dx^2} - \frac{d}{dx} \left( N \frac{du}{dx} \right) = 0.$$

where  $F_A$  denotes the axial force  $M$  is the bending moment,  $N$  is applied load and  $u$  denotes the deflection field. The bending moment in terms of

generalized displacement is given by

$$(3) \quad M = -EI \frac{d^2u}{dx^2} + (e_0a)^2 \frac{d}{dx} \left( N \frac{du}{dx} \right).$$

where  $E$  is the Young's modulus,  $I$  is the second moment of area,  $\mu = (e_0a)^2$  is the nonlocal parameter in which  $e_0$  is a constant specific to each material and  $a$  is granular distance. Assuming the axial compressive load  $N = \widehat{N}$  to be constant and using equation (2-3), the above equations reduces to

$$(4) \quad -EI \frac{d^4u}{dx^4} + (e_0a)^2 N \frac{d^4u}{dx^4} - N \frac{d^2u}{dx^2} = 0$$

Non-dimesionalized form of the above equation is

$$(5) \quad \frac{d^4u}{dX^4} - \omega^2 \frac{d^2u}{dX^2} = 0$$

where

$$(6) \quad X = \frac{x}{l}, \omega^2 = \left( \frac{N}{N \mu^2 - EI/l^2} \right)$$

The boundary conditions for single walled carbon nanotube in case of simply supported (SS) and clamped clamped (CC) are

$$(7) \quad \left. \begin{aligned} u(x) = M(x) = 0, \text{ at } x = 0, l \\ u(x) = u'(x) = 0, \text{ at } x = 0, l \end{aligned} \right\}$$

The solution of equation (5) is obtained using appropriate end supports (7).

### 3. SOLUTION OF THE PROBLEM

Numerical solution of the formulated problem (5) is obtained using Galerkin's approach. A simple MATLAB code is generated to solve the system of equations. Although the analytical solutions of the problem under study are available in the literature, numerical method is applied to reduce computational efforts. Solution of equation (5) by Galerkin's method is expressed according to [14] as

$$(8) \quad u(X) = \sum_{j=-2}^{n+2} c_j B_j(X)$$

where  $c_j$  are the node parameters to be calculated using specified end conditions (7) and  $B_j(X)$  are the quintic B-splines applied as a weight function and are defined in [27] as follows

$$(9) \quad B_i(z) = (1/h^5) \begin{cases} (z - z_{i-3})^5 & z \in [z_{i-3}, z_{i-2}) \\ (z - z_{i-3})^5 - 6(z - z_{i-2})^5 & z \in [z_{i-2}, z_{i-1}) \\ (z - z_{i-3})^5 - 6(z - z_{i-2})^5 + 15(z - z_{i-1})^5 & z \in [z_{i-1}, z_i) \\ (z_{i+3} - z)^5 - 6(z_{i+2} - z)^5 + 15(z_{i+1} - z)^5 & z \in [z_i, z_{i+1}) \\ (z_{i+3} - z)^5 - 6(z_{i+2} - z)^5 & z \in [z_{i+1}, z_{i+2}) \\ (z_{i+3} - z)^5 & z \in [z_{i+2}, z_{i+3}) \\ 0 & \text{otherwise} \end{cases}$$

$i = 0, 1, 2, \dots, n$ . The solution space  $0 \leq z \leq 1$  is discretized in to a mesh of uniform length  $h = z_{i+1} - z_i$  such that  $0 = z_0 < z_1 < z_2 < \dots < z_n = 1$ . When applying the Galerkin function, all the  $B_i(z)$ 's should vanish on the boundary where the end conditions are applied, but some of  $B_i(z), i = -2(1)2, (n-2)(1)(n+2)$  do not vanish and thus it is required to redefine them so that they fulfill the Dirichlet's type end conditions at boundary. A new set of quintic B-splines satisfying the boundary  $u(0) = u(1) = 0$  are given according to [14] as

$$(10) \quad \tilde{B}_j(X) = \begin{cases} B_j(X) - \frac{B_j(X_0)}{B_{-2}(X_0)}B_{-2}(X), & j = -1(1)2 \\ B_j(X), & j = 3(1)(n-3) \\ B_j(X) - \frac{B_j(X_n)}{B_{n+2}(X_n)}B_{n+2}(X), & j = (n-2)(1)(n+1) \end{cases}$$

Applying this new basis function to solve (4), we get

$$(11) \quad \int_0^1 [u^{(4)}(X) - \omega^2 u^{(2)}(X)] \tilde{B}_j(X) dX = 0$$

Integrating each term of the equation (11) and applying boundary conditions (6), we get a system of simultaneous equations that determine the approximate value of  $u(X)$  as follows

$$(12) \quad [a_{ij}]C = [b_i]$$

$$\begin{aligned} \text{where } a_{ij} &= \int_0^1 \left[ -\frac{d^3}{dx^3} \tilde{B}_i(X) - \frac{d}{dx} \tilde{B}_i(X) \right] dx + \left[ \frac{d}{dx} \tilde{B}_j(X) \right]_{X=0} \tilde{B}_j''(X)_{X=0} \\ &- \left[ \frac{d}{dx} \tilde{B}_j(X) \right]_{X=1} \tilde{B}_j''(X)_{X=1}; i = -1(1)n+1, j = -1(1)n+1 \\ b_i &= \int_0^1 \left[ -\frac{d^3}{dx^3} \tilde{B}_i(X) + \frac{d}{dx} \tilde{B}_i(X) \right]; i = -1(1)n+1 \\ &\text{and} \\ C &= [C_{-1}C_0C_1 \dots \dots \dots C_n C_{n+1}]^T \end{aligned}$$

#### 4. RESULTS AND DISCUSSIONS

The lowest buckling load/strain for SWCNT is found out and the outputs are plotted graphically. The values of material parameters employed in numerical results for chiral single walled carbon nanotube are considered as

$$E = 1.0 \text{ TPa}, I = (\pi r^4)/4,$$

where  $r$  is the radius of the nanotube taken as 0.5 nm. The effect of slender ratio (length to diameter ratio) on critical strain ratio is illustrated in figure 1. Different values of non-local parameter are used to observe the buckling behavior of nanotubes with respect to different slender ratios. It can be seen that critical load variation is more pronounced for short carbon nanotubes. In addition, the nonlocal parameter has a significant impact on smallest buckling load and reduces as the value of this parameter increases. It is important to note that the critical load ratio approaches to unity for larger carbon nanotube. It is worth mentioning that the variations in buckling load for smaller slender ratios is nonlinear, this may be due to the reason that

the nanotubes are more stiffer for smaller slender ratios. Similar variations are observed in (19).

5. FIGURE CAPTION POSITION

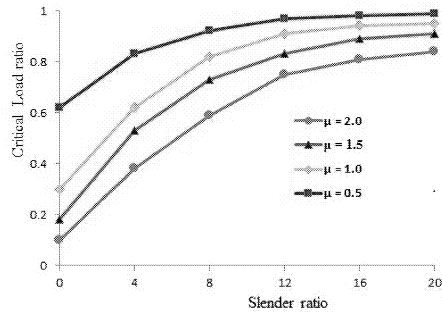


FIGURE 1. Variation in critical buckling load with length parameter

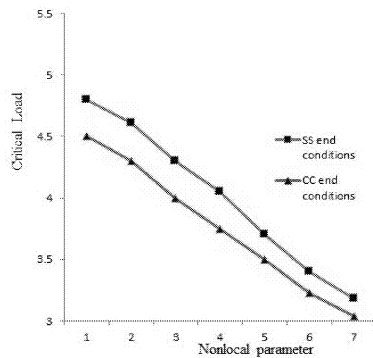


FIGURE 2. Variation in critical buckling load with nonlocal parameter

6. CONCLUSIONS AND FUTURE SCOPE

The present work studies the buckling response of single walled carbon nanotube. The formulation of governing equations is obtained with appropriate end conditions and an efficient mathematical technique is applied to determine the results. The findings show the relationship of critical buckling load with length parameter, nonlocal parameter and end conditions. Further, the present study illustrates the use of quintic splines to solve the governing differential equations and to analyze the behavior of nanostructures. Since the buckling nature of nanostructures help in determining their stability, this study will help in designing more efficient nano-electronics and nano-composites systems.

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