BUCKLING ANALYSIS OF A SIMPLY SUPPORTED SINGLE-WALLED CARBON NANOTUBE USING NONLOCAL CONTINUUM MODEL AND LAPLACE TRANSFORM

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Abstract: Using nonlocal continuum model we have obtained expressions for transverse deflection and buckling load for a simply supported single-walled carbon nanotube for different aspect ratios (L/d). We used Laplace transform method to calculate results. We found that these results are in good agreement with the exact analytical solution and the small scale coefficient has a noticeable effect on the buckling load of the carbon nanotube (CNT). This shows that Laplace transform method can be used in investigating different boundary problems on CNTs with nonlocal effects.

Keywords: buckling; nonlocal continuum model; single-walled carbon nanotube; Laplace transform

1. Introduction:

The role of carbon nanotubes (CNTs) in modern technologies is becoming increasingly significant because of their outstanding mechanical [1,2], electrical [3] and thermal properties [4]. These superior properties of CNTs make them preferable candidates for a number of applications such as building different kinds of nanodevices in nanoelectromechanical, micro-electromechanical and many other systems. Before using CNTs for practical applications its mechanical properties should be known. For this many researchers have performed experiments but its mechanical properties have not yet fully understood. Since performing experiments at nanoscale are very expensive and also difficult to control, therefore, as an alternative, researchers perform various simulations such as molecular dynamics [5], molecular mechanics [6], density functional theory [7] to study their mechanical properties. Although the results of the simulation methods are in good agreement with the experimental results, these methods require considerable time and computational effort. It is found that the continuum models can give satisfactory results in describing mechanical properties of CNTs [5]. Further, the local continuum model is suitable for studying mechanical properties of CNTs at length scale greater than 100 nm [8]. However, its applicability at small length scale (less than 100 nm) is questionable [9] because they do not take into account the intrinsic size dependence of the CNTs. At small length scale the micro structure of the material, such as lattice spacing between individual atoms, becomes important and cannot be ignored. Hence, an appropriate continuum model is needed to properly investigate the effect of small scale coefficient in the mechanical properties of CNTs. This can be solved by using nonlocal continuum model proposed by Eringen [10].

The nonlocal continuum model has been successfully used for bending, buckling and vibration of CNTs and other nanosized structures. Sudak [8] investigated the buckling behaviour of multi-walled CNTs by incorporating the van der Waals forces and the effects of small scale coefficient. This work concluded that the small scale coefficient contributes significantly into the critical axial strain of buckling and cannot be neglected. Wang et al. [11] derived the expressions for buckling load of CNTs using nonlocal continuum model and Euler–Bernoulli beam theory. They showed that when small scale effect is considered the buckling load becomes smaller.

In this work, we have used nonlocal continuum model and Euler-Bernoulli beam theory to investigate the small scale effect on the buckling behaviour of a simply supported single-walled carbon nanotube (SWCNT). We have derived an expression for transverse deflection of the CNT using Laplace transform method. We have also obtained an expression for buckling load and calculated its numerical values for CNTs having different aspect ratios (L/d) for various small scale coefficients (e_0a) as shown in table 1. Further, we have plotted the first and second buckling deflection modes in figure 2.

2. Nonlocal continuum model for buckling analysis of a simply supported single-walled CNT:

In nonlocal elastic theory, the stress at a reference point in the body depends on strains at all points of the body [10,11]. This is based on the atomic theory of lattice dynamics and some experimental observations on phonon dispersion. In this approach, the intrinsic size scale is included in the constitutive equations as a material parameter [11,12]. If the effects of strains at points other than the point considered are neglected, it reduces to the classical or local theory of elasticity. The constitutive equation of a linear, homogeneous, isotropic, nonlocal elastic solid with zero body force are given by [10,11]

$$\sigma_{ij}(\boldsymbol{x}) = \int_V \alpha(|\boldsymbol{x}-\boldsymbol{x}'|,\tau) C_{ijkl}\varepsilon_{kl}(\boldsymbol{x}')dV(\boldsymbol{x}');\;\; \forall \boldsymbol{x}\in V \tag{1}$$

where σ_{ij} and ε_{kl} are stress and strain tensors respectively, C_{ijkl} is the elastic modulus tensor of classical isotropic elasticity, the scalar function $\alpha(|\boldsymbol{x}-\boldsymbol{x}'|,\tau)$ is the attenuation function, which serves to incorporate the nonlocal effects at the reference point $\boldsymbol{x}$ produced by local strain at the source $\boldsymbol{x}$' into the constitutive equation, and $\tau = \mathrm{e_0 a}/l$, where $\mathrm{e_0}$ is a constant appropriate to each material, a is an internal characteristic length (e.g., length of *C-C* bond, lattice parameter, granular distance), and l is an external characteristic length (e.g., crack length, wavelength). The value of $\mathrm{e_0}$ needs to be determined from experiments or matching dispersion curves of plane waves with those of atomic lattice dynamics. The integral is over the entire volume V occupied by the elastic body.

The equivalent differential form of equation (1) is written in one-dimensional case as [11,12]

$$\left[1-(\mathrm{e_0 a})^2\frac{d^2}{dx^2}\right]\sigma(x) = E\varepsilon(x) \tag{2}$$

where E is the Young's modulus of the CNT. We use nonlocal continuum model and Euler-Bernoulli beam theory to study buckling behaviour of a cylindrical simply supported SWCNT of length L and diameter d. The equilibrium equation for the bending moment (M) on the one-dimensional structure subjected to an axial compression F is

$$\frac{dM}{dx} = \mathrm{F}\frac{dy}{dx} \tag{3}$$

where y is the transverse deflection of the CNT. Differentiating the above equation with respect to x we get

$$\frac{d^2M}{dx^2} = \mathrm{F}\frac{d^2y}{dx^2} \tag{4}$$

For small bending, the bending moment (M) and the axial strain (ε) of the CNT are given by [10]

$$M(x) = \int_A \sigma(x)zdA \qquad \text{and} \qquad \varepsilon(x) = -z\frac{d^2y}{dx^2} \tag{5}$$

Using equation (5) in equation (2) we get

$$\left[1-(\mathrm{e_0 a})^2\frac{d^2}{dx^2}\right]M(x) = -EI\frac{d^2y}{dx^2} \tag{6}$$

where EI is the bending rigidity of the CNT. The expression for M is obtained by using equation (4) in equation (6)

$$M(x) = -[EI-\mathrm{F}(\mathrm{e_0 a})^2]\frac{d^2y}{dx^2} \tag{7}$$

At any point x, M is also given as [13]

$$M(x) = \mathrm{F}y - M(0)$$

where $M(0)$ is the bending moment at the supported end ($x = 0$). Using the above expression in equation (7) we have

$$\mathrm{F}y - M(0) = -[EI-\mathrm{F}(\mathrm{e_0 a})^2]\frac{d^2y}{dx^2}$$

or,
$$\frac{d^2y}{dx^2} + \frac{\mathrm{F}y}{EI-\mathrm{F}(\mathrm{e_0 a})^2} = \frac{M(0)}{EI-\mathrm{F}(\mathrm{e_0 a})^2}$$

or,
$$\frac{d^2y}{dx^2} + \xi^2 y = \mathrm{K} \tag{8}$$

where

$$\xi = \sqrt{\frac{\mathrm{F}}{EI-\mathrm{F}(\mathrm{e_0 a})^2}} \tag{9a}$$

and

$$\mathrm{K} = \frac{M(0)}{EI-\mathrm{F}(\mathrm{e_0 a})^2} \qquad \text{9b)}$$

Now applying Laplace transform [14] to equation (8) we get

$$L\{\frac{d^2y}{dx^2}\} + \xi^2 L\{y\} = \mathrm{K}L\{1\}$$

or,
$$s^2 L\{y\} - sy(0) - y'(0) + \xi^2 L\{y\} = \frac{\mathrm{K}}{s} \tag{10}$$

For a simply supported CNT the boundary conditions are

$$y(0) = M(0) = 0 \tag{11a}$$

$$y(\mathrm{L}) = M(\mathrm{L}) = 0 \tag{11b}$$

Using boundary condition (11a) in equations (9b) and (10) we obtain

$$(s^2 + \xi^2)L\{y\} = y'(0)$$

or,
$$L\{y\} = \frac{y\prime(0)}{(s^2+\xi^2)} = \frac{\Theta}{\xi}\frac{\xi}{(s^2+\xi^2)}$$

where $\Theta = y'(0)$. Applying inverse Laplace transform to the above equation we get

$$y(x) = \frac{\Theta}{\xi}\sin\xi x$$

or,
$$y(x) = \mathrm{C}\sin\xi x \tag{12}$$

where $\mathrm{C} = \frac{\Theta}{\xi}$. Equation (12) represents the transverse deflection of a CNT under buckling. Using boundary condition (11b) in equation (12) we get

or,
$$\mathrm{C}\sin\xi\mathrm{L} = 0$$

or,
$$\sin\xi\mathrm{L} = 0 \quad (\text{since } \mathrm{C} \neq 0)$$

The above condition implies that

$$\xi\mathrm{L} = n\pi$$

or,
$$\xi = \frac{n\pi}{\mathrm{L}} \quad \text{for } n = 0, 1, 2, 3, \ldots \tag{13}$$

Squaring equation (13) on both sides and then using equation (9a), we obtain the buckling load for the CNT as

$$\mathrm{F} = \frac{\frac{n^2\pi^2}{\mathrm{L}^2}EI}{1+(e_0\mathrm{a})^2\frac{n^2\pi^2}{\mathrm{L}^2}} \tag{14}$$

This shows that the value of F increases with EI but decreases with L^2 and $(\mathrm{e}_0\mathrm{a})^2$. When $\mathrm{e}_0\mathrm{a} = 0$ then equation (14) gives the same expression for the buckling load of a local simply supported CNT. Now, substituting the expression of ξ from equation (13) in equation (12) we get

$$y(x) = \mathrm{C}\sin\frac{n\pi x}{\mathrm{L}} \tag{15}$$

Equation (15) represents the buckling deflection mode for a simply supported CNT.

3. Results and discussion:

We consider SWCNTs with different lengths (L = 10 - 20 nm), each having the same diameter (d = 1 nm) and $E = 1$ TPa [15]. Using equation (14) we have calculated the numerical values of F for CNTs having different aspect ratios ($\mathrm{L/d} = 10, 12, 14, 16, 18, 20$) for various small scale coefficients ($\mathrm{e}_0\mathrm{a}$ = 0.0, 0.5 1.0, 1.5, 2.0 nm) at $n = 1$ and $n = 2$ as shown in table 1.

Table 1: Buckling loads F (nN) for a simply supported SWCNT at $n = 1$ and $n = 2$.

	$\mathrm{e}_0\mathrm{a}$ (nm)					$\mathrm{e}_0\mathrm{a}$ (nm)				
	0.0	0.5	1.0	1.5	2.0	0.0	0.5	1.0	1.5	2.0
L/d	F (nN) ($n = 1$)					F (nN) ($n = 2$)				
10	4.8447	4.7280	4.4095	3.9643	3.4734	19.3788	17.6380	13.8937	10.2627	7.5137
12	3.3644	3.3077	3.1486	2.9149	2.6405	13.4575	12.5943	10.5619	8.3233	6.4186
14	2.4718	2.4411	2.3533	2.2202	2.0574	9.8871	9.4131	8.2295	6.8037	5.4756
16	1.8925	1.8744	1.8222	1.7414	1.6396	7.5698	7.2888	6.5584	5.6199	4.6818
18	1.4953	1.4840	1.4511	1.3994	1.3329	5.9811	5.8043	5.3315	4.6942	4.0212
20	1.2112	1.2037	1.1820	1.1475	1.1024	4.8447	4.7280	4.4095	3.9643	3.4734

The results are then compared with that of Ref. 16. We found that our results are in very good agreement with them for $n = 1$. In figures 1(a) and 1(b) we have plotted aspect ratio (L/d) versus buckling load (F) at $n = 1$ and $n = 2$ respectively. Using equation (15), we plot x/L versus y/C for a CNT with $\mathrm{L} = 14$ nm at $n = 1$ and $n = 2$, which is shown in figure 2. From figure 1 we observe the followings:

* For a given aspect ratio the value of F decreases as the small scale coefficient increases for both the first ($n = 1$) and second ($n = 2$) modes of buckling. This shows the significant effect of small scale coefficient on the buckling behaviour of CNT.

* For a given value of small scale coefficient the value of buckling load decreases with increasing the value of aspect ratio and it is more for the case of $n = 2$ than that of $n = 1$. This shows that small scale effect is more noticeable for CNTs with shorter lengths. This is because the nonlocal effect is definitely large within short distance in substances.

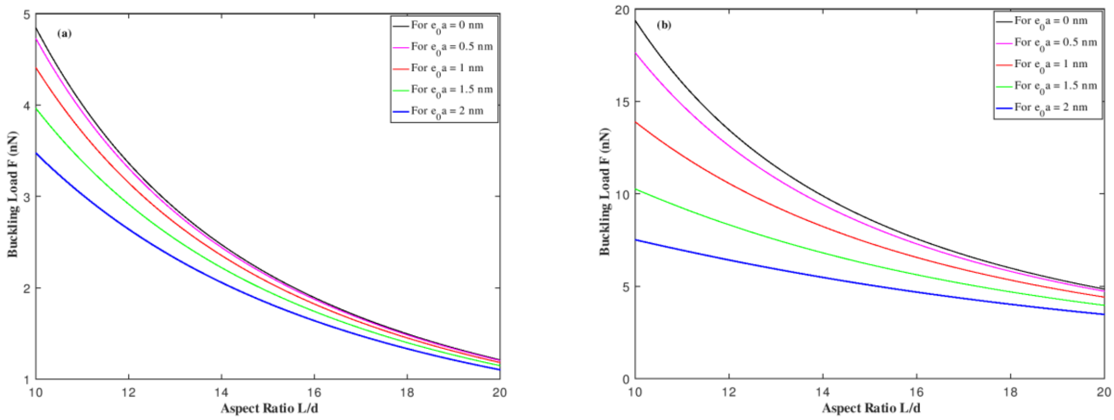

Figure 1: Aspect ratio (L/d) versus load (F) at (a) $n = 1$ and (b) $n = 2$.

From figure 2 it can be seen that for the first buckling mode there is one antinode, located at the mid-point of the CNT whereas for the second buckling mode there are two asymmetric antinodes, located at one-fourth and three-fourth of the total length of the CNT.

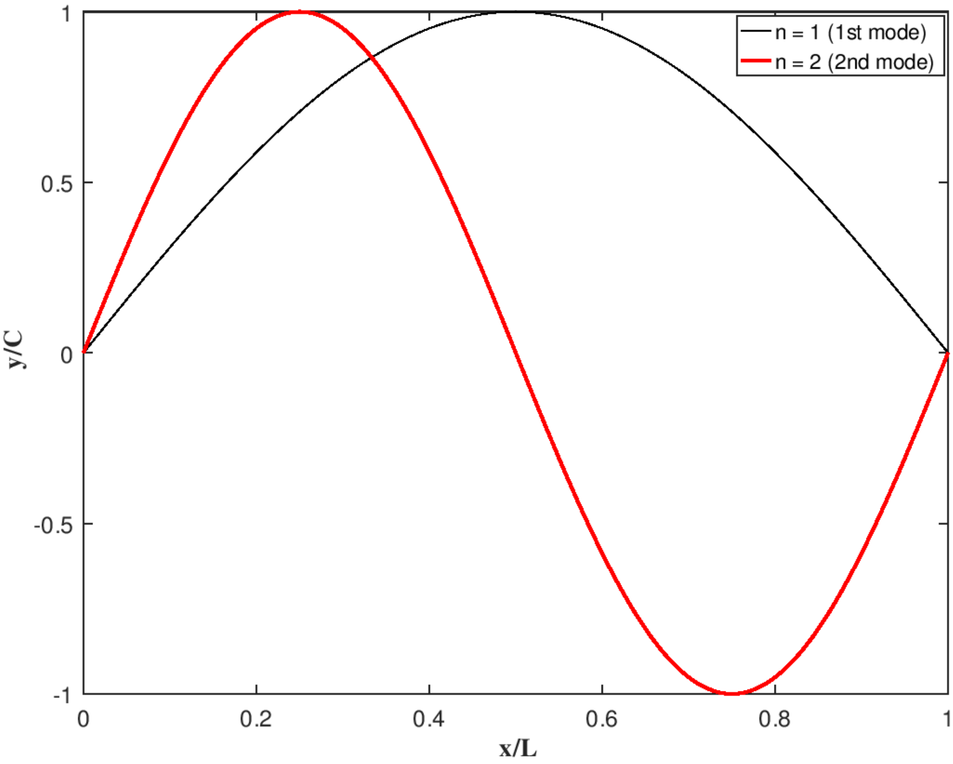

Figure 2: The first and second buckling modes of a CNT with L = 14 nm.

4. Conclusion:

We have derived the expressions for transverse deflection and buckling load for a simply supported single-walled CNT using nonlocal continuum model. Using Laplace transform method we have obtained the transverse deflection of the CNT. The results obtained from Laplace transform gives exactly the same value as that of analytical method. Moreover the Laplace transform method is simpler than that of the analytical method. We found that the small scale effect is more noticeable for CNT with shorter length for the case of simply supported single-walled CNT. Further, the small scale effect on the buckling load is more with the higher mode. Our results will be helpful in investigating more complicated boundary problems on CNTs with nonlocal effects.

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