

Buckling of multi wall carbon nanotube cantilevers near graphite sheets using monotone solution method*¹ Mohammad Ghalambaz, ²Aminreza Noghrehabadi, ³Amir vosough¹ Department of Mechanical Engineering, Dezful Branch, Islamic Azad University, Dezful, Iran² Department of Mechanical Engineering, Ahvaz Branch, Islamic Azad University, Ahvaz, Iran.³ Young researchers club, Mahshahr Branch, Islamic Azad University, Mahshahr, Iran.*m.ghalambaz@gmail.com

Abstract- In this paper, a monotone positive solution is studied for buckling of a distributed model of multi walled carbon nanotube (MWCNT) cantilever in the vicinity of thin and thick graphite sheets subject to intermolecular forces. In the modeling of intermolecular forces van der Waals forces are taken into account. A hybrid nano-scale continuum model based on Lennard–Jones potential is applied to simulate the intermolecular force-induced deflection of MWCNT. A positive monotone solution base on Green’s function in the form of a nonlinear iterative integral is introduced, to obtain a solution for deflection of MWCNT cantilevers. In order to determine the accuracy of presented method, the results are compared with numerical results of a boundary value method as well as other methods reported in the literature. The results are show the monotone iterative solution is stable and converged to numerical results with a few iterations. The results of present work are useful to prove the stability and convergence of Green’s function to deal with deflection of nano cantilever switches in future works and simplifications.

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1. Introduction

Multi walled carbon nanotubes (MWCNTs) have attracted considerable attention among other nanomaterials. These novel materials can usually be visualized as nano-scale concentric cylinders rolled up by graphene sheets. MWCNTs are produced by different techniques, such as chemical vapor deposition, laser ablation, and arc discharge. It has been reported that the stiffness, flexibility and strength of carbon nanotubes are much higher than the conventional materials [1, 2]. Furthermore, nanotubes can provide various ranges of conductive properties depending on their atomic and geometrical structure [3, 4]. The extraordinary properties of MWCNTs have motivated worldwide engineers to explore their applications in different fields.

Some nano scale actuator systems have been constructed based on single carbon nanotubes and nanowires. Nanotube nanotweezers made by attaching two individual nanotubes onto a sharp tip was reported capable of nano manipulation and electrical detection, which was actuated by electrostatic forces between the nanotubes [5]. A low-friction, nanoscale, linear bearing from an individual multi-wall carbon nanotube was reported [6]. Static and dynamic mechanical deflections was electrically induced in cantilevered multi-wall carbon nanotubes in a transmission electron microscope (TEM) [7], while double-clamped, suspended, single nanotube and nanowire behaved as high frequency resonators [8, 9]. Nanotube-based, electrically driven, torsional

actuators have also been reported [10, 11]. These studies showed the potential to construct nano scale actuation systems based on individual nanostructures. Also, With recent growth in nanotechnology, MWCNTs are increasingly used in developing atomic force microscope (AFM) probes [1,3, 12,13] and nano-electromechanical system (NEMS) switches [14–16].

Consider a typical cantilever MWCNT probe/switch suspended near graphite surface with a small gap in between. As the gap decreases from micro to nano-scale, the van der Waals interaction deflects MWCNT to the surface. When the separation is small enough, nanotube buckles onto graphite. A reliable trend to simulate the deflection of MWCNT interacting with extremely large number of graphite atoms is to apply nano-scale continuum models. In our previous work [17] we utilized a hybrid continuum model to investigate the molecular force-induced buckling of the cantilever freestanding MWCNT probes/actuators suspended over graphite. Then buckling of multi walled carbon nanotube (MWCNT) probes/actuators in the vicinity of thin and thick graphite was carried out for the first time. The governing equation of the distributed model leads to a forth order nonlinear differential equation. Because of the nonlinearity of governing equations of distributed model on the deflection of nanotubes obtaining an analytical solution for this type of nanotubes is hard and complicated. The obtained non dimensional differential equation for large number of graphene

layers is the same as the non dimensional governing differential equation of nano cantilever beams with rectangular cross section subject to Casimir effect and neglecting electrical force [18]. Therefore the methods which are used to obtain buckling and pull-in parameters of nano cantilevers with rectangular cross section maybe usable to obtain a solution on the buckling of carbon nano tube cantilevers. In order to study the deflection and pull-in parameters of nano-cantilever beams with rectangular cross section, some investigators assumed the electrostatic and intermolecular forces uniform along the beam [19-23] and some of them, used distributed models [18,24,25]. Some researchers [17, 18,26] tried to find semi analytical solutions for this problem using Adomian decomposition method and some others tried to find approximate solutions [18-24, 25,27]. Most of the approximate solutions (i.e. solution of distributed model) are base on Green’s function and then some simplifications [17, 18, 24, 25]. But they never attempt to solve obtained Green’s function directly with out any simplifications. Existence of monotone positive solution for a class of beam equations has been investigated by previous researchers [28-36]. Unfortunately the governing equation of nano-beam can’t be categorized in any of the maintained works (i.e. [28-36]). Abaydan [17] and Ramezani [24, 25] used Greens function method with a simple second order polynomial as shape function to obtain deflection and pull-in parameters of MWCNT cantilevers and nano beam cantilevers, respectively. However, their results on the calculating of deflection in comparison with numerical results are acceptable but their accuracy is not perfect.

In the present work, a monotone iterative solution basis on Green’s function is introduced and solved directly to obtain buckling of MWCNT cantilevers. The results are compared with numerical results as well as simplified Greens function method those in [17] and with power series results in [26].

2. Mathematical model

Figure 1 shows a schematic of a typical freestanding MWCNT near a surface consisted of N graphene layers, with interlayer distance $d = 3.35\text{\AA}$. The length of MWCNT is L , the mean value of their radius is R_w , the number of walls of nanotube is N_w , and the gap between MWCNT and the surface is D .

Elastostatic domain

Based on continuum mechanics, a MWCNT is modeled by concentric cylindrical tubes. Young’s modulus of MWCNT, E_{eff} , is typically 0.9 - 1.2 TPa [37] and the cross-sectional moment of inertia I is equal to $\pi (R_o^4 - R_i^4)/4$ [17]. By applying the Euler theory and neglecting the effect of large displacement

(finite kinematics) for $L/D \gg 10$ [22-23], the governing equation of a cantilever MWCNT can be defined as following boundary value differential equation [17]

$$E_{eff} I \frac{d^4 U}{dX^4} = q_{vdw} (D - U) \tag{1-a}$$

subject to geometrical boundary conditions at fixed end

$$U(0) = \frac{dU}{dX}(0) = 0 \tag{1-b}$$

and natural boundary conditions at free end

$$\frac{d^2 U}{dX^2}(L) = \frac{d^3 U}{dX^3}(L) = 0 \tag{1-c}$$

where X is the position along MWCNT measured from the clamped end, U is the deflection of MWCNT and q_{vdw} is the intermolecular force per unit length of MWCNT. According to our previous work [17], q_{vdw} base on double-volume integral of Lennard–Jones potential in [38-40] and some simplification can be represented as follow

$$q_{vdw} = \begin{cases} \frac{C_6 \sigma^2 \pi^2 N_w R_w}{d(D-U)^4} & \text{For large number of layers} \\ \frac{4C_6 \sigma^2 \pi^2 N N_w R_w}{d(D-U + Nd/2)^4} & \text{For small number of layers} \end{cases} \tag{2}$$

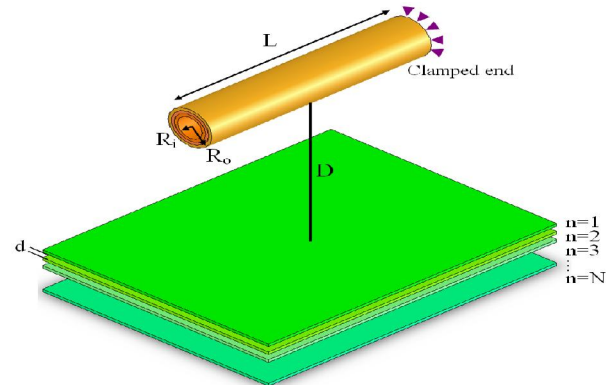


Figure. 1. Schematic of a MWCNT over graphite ground plane.

In the above equation, $C_6 = 15.2 eV \text{\AA}^6$ is the attractive constants for the carbon - carbon interaction, [41] and $\sigma \approx 38 \text{nm}^{-2}$ [38] is the graphene surface density. By substituting (2) in (1) and using the following substitutions the dimensionless form of (1) can be obtained.

$$x = \frac{X}{L}, \quad u = \begin{cases} \frac{U}{D} & (n=4) \\ \frac{U}{D + Nd/2} & (n=5) \end{cases} \tag{3}$$

$$f_n = \begin{cases} \frac{C_6 \sigma^2 \pi^2 N_w R_w L^4}{d E_{eff} I D^5} & (n = 4) \\ \frac{4C_6 \sigma^2 \pi^2 N N_w R_w L^4}{E_{eff} I (D + Nd/2)^6} & (n = 5) \end{cases}$$

In the following text, $n = 4$ and $n = 5$ correspond to the large number and small number of graphene layers, respectively. These transformations yield,

$$\frac{d^4 u}{dx^4} = \frac{f_n}{(1-u(x))^n} \quad (4-a)$$

$$\begin{aligned} u(0) = u'(0), \quad \text{at } x = 0, \quad \text{and} \\ u''(1) = u'''(1) = 0, \quad \text{at } x = 1 \end{aligned} \quad (4-b)$$

In all equations, prime denotes differentiation with respect to x .

3. Mathematical approach

According to Green's function method, the response of a system to an arbitrary load can be constructed using the load distribution and the response to a concentrated load [25-27]. The concentrated load at $x = s$ is modeled using Dirac delta function $\delta(x-s)$. By replacing the right hand side of equation (4-a) with $\delta(x-s)$, and u with G , the following is obtained

$$\frac{d^4 G}{dx^4} = \delta(x-s) \quad (5-a)$$

$$\begin{aligned} G(0) = G'(0) = 0, \quad \text{at } x = 0 \\ \text{and } G''(1) = G'''(1) = 0, \quad \text{at } x = 1 \end{aligned} \quad (5-b)$$

which models a cantilever nano-beam with a concentrated load at $x = s$. The solution to this problem (Green's function) is

$$G(x) = \begin{cases} k_0 x^3 + k_1 x^2 + k_2 x + k_3 & 0 \leq x \leq s \\ p_0 x^3 + p_1 x^2 + p_2 x + b_3 & s \leq x \leq 1 \end{cases} \quad (6)$$

The coefficients k_i and p_i in (6) are unknown constants. By imposing the boundary conditions at $x=0$ and $x=1$ we obtain

$$G(x) = \begin{cases} k_0 x^3 + k_1 x^2 & 0 \leq x \leq s \\ p_2 x + p_3 & s \leq x \leq 1 \end{cases} \quad (7)$$

Equation (7) contains four unknown constants (k_0, k_1, p_2, p_3). These constants can be determined from remaining conditions. Three conditions comes from

continuity of nano-beam shape and its first and second derivatives at s , so we have

$$G(s^-) = G(s^+), \quad G'(s^-) = G'(s^+), \quad G''(s^-) = G''(s^+) \quad (8)$$

The fourth condition comes from integrating (5-a) across the point s to obtain the following

$$G'''(s^+) - G'''(s^-) = 1 \quad (9)$$

where the minus and plus indicate the left and right of s , respectively. By applying (8) and (9) on (7) we obtain

$$G(x, s) = \frac{1}{6} \begin{cases} s^2(3x-s) & \text{if } 0 \leq x \leq s \\ x^2(3s-x) & \text{if } s \leq x \leq 1 \end{cases} \quad (10)$$

Now, the derived Green's function is used to construct a solution to our non uniformly distributed loading problem. Multiplying (5-a) by u and (4-a) by G , subtracting the two equations, and integrating from $x = 0$ to $x = 1$, leads to

$$\int_0^1 \left(G \frac{d^4 u}{dx^4} - u \frac{d^4 G}{dx^4} \right) dx = \int_0^1 (FG - u\delta) dx \quad (11)$$

Integrating the left-hand side of (11) by parts and applying the boundary conditions (4-b) and (5-b), then using symmetric property of $G(x, s)$ then renaming the variables, leads to

$$u(x) = \int_0^1 G(x, s) \left(\frac{\alpha}{(1-u(s))^n} \right) ds \quad (12)$$

This is the integral representation of the nonlinear differential equation (4). Unfortunately, (12) is an implicit integral equation. This equation can be written in an iterative form [29, 42] as

$$\begin{aligned} u^{n+1}(x) = \frac{1}{6} \int_0^x s^2(3x-s) \left(\frac{\alpha}{(1+u^n(s))^n} \right) ds \\ + \frac{1}{6} \int_x^1 x^2(3s-x) \left(\frac{\alpha}{(1+u^n(s))^n} \right) ds \end{aligned} \quad (13)$$

The iterative solution can start from an initial guess. Hence, we take $u_0(x) = x/3$ and $u_0(x) = 0$. In the next section, (4) will be solve by using (13) for $f_n^* = 0.5$ and also for a range of f_n^* . The results of monotone solution are compared with results of boundary value solution.

4. Results

The first iterative solution of equation (4) starting from $u_0(x) = 0$ leads to the following analytical equation

$$U^1(x) = \alpha \frac{x^2}{4} - \alpha \frac{x^3}{6} + \alpha \frac{x^4}{24} \quad (14)$$

Symbolic calculation of second and higher iterations of $u(x)$ is very complicated so numerical integration is needed. In order to calculate integrals of (13) numerically, the adaptive Simpson quadrature integration method is used. In order to verify convergence and convergence rate of the monotone method, (4) solved for with $f_n^* = 0.5$ for small and large number of graphite layers which are used in [17]. Figure (2) and figure (3) show the centerline deflection of MWCNT cantilever nanotube for $f_n^* = 0.5$ and small number of graphite layers, by using monotone method starting from $u_0(x) = 0$ and $u_0(x) = x/3$, respectively. In these figures the results of different iterations are compared with numerical solution. Table 1 compares the tip deflection of nanotube cantilever obtained using monotone solution (by different starting values) with numerical results and Adomian series size of 10 those on [17]. Numerical results are obtained using a combination of trapezoid as base scheme and Richardson extrapolation as enhancement scheme [43, 44].

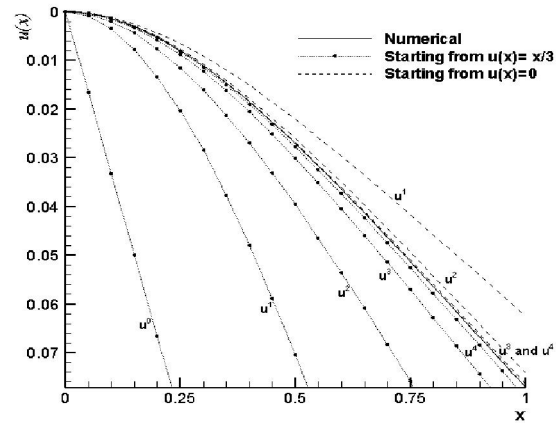


Figure 2: Buckling of MWCNT cantilever with large number of graphite sheets (i.e. $n = 4$) when $f_n = 0.5$ for to different iterations of monotone solutions and different starting values.

It can be seen in table 1 the accuracy of monotone solution with starting from $u_0(x) = 0$ is more than those starting from $u_0(x) = x/3$. Therefore, $u_0(x) = 0$ is chosen in later calculations. Figure (4) shows the variation of cantilever tip deflection as a function of f_n^* for large numbers of graphite layers and small number of graphite layers. Figure 4 compares centerline buckling of nanotube obtained by monotone method with numerical results as well with Green's function and Adomian those on [17, 26] and series solution [26].

Table 1: the variation of tip deflection of a typical MWCNT cantilever obtained using different iterations and different start values for $f_n = 0.5$. The iterative solution converges to the numerical solution as the number of the iterations increase.

Iteration	n=4		Tip deflection by numerical method	n=5		Tip deflection by numerical method
	Tip deflection by using monotone solution with $U_0(x)=0$	Tip deflection by using monotone solution with $U_0(x)=x/3$		Tip deflection by using monotone solution with $U_0(x)=0$	Tip deflection by using monotone solution with $U_0(x)=x/3$	
1	0.0625	0.20564	0.07719	0.0625	0.28125	0.083234
2	0.074073	0.114582		0.077335	0.189006	
3	0.076515	0.086002		0.081496	0.125078	
4	0.077044	0.07915		0.082717	0.097114	

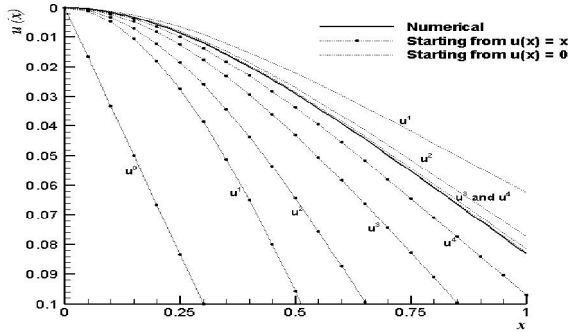


Figure 3: Buckling of MWCNT cantilever with small number of graphite sheets (i.e. $n = 5$) when $f_n = 0.5$ for to different iterations of monotone solutions and different starting values.

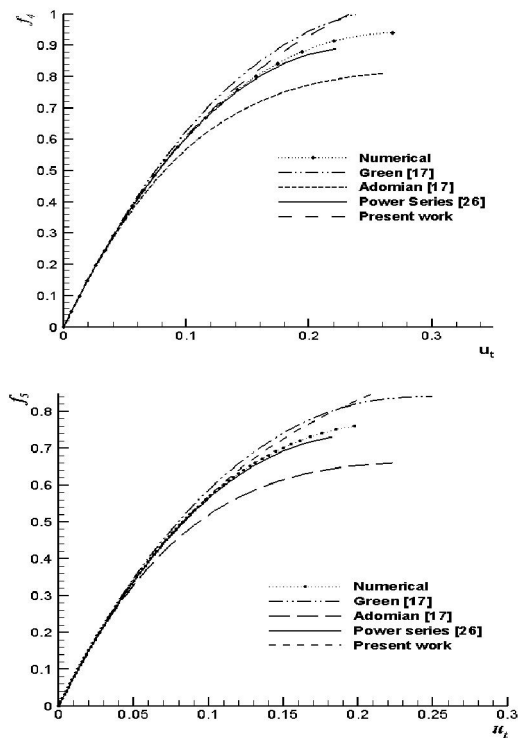


Figure 4. Comparing the tip buckling of MWCNT cantilever obtained by monotone solution with $u_0(x)=0$ with other methods for (a) Large number of graphite layers (i.e. $n=4$) (b): Small number of graphite layers (i.e. $n = 5$)

5. Conclusions

In this paper, a monotone positive solution is studied for buckling of MWCNT cantilevers with small and large number of graphite layers subject to distributed electrostatic force and van der Waals attractions. The governing differential equation is fourth order and nonlinear due to the inherent of the van der Waals and electrostatic interactions. The nonlinear differential equation is transformed into an

implicit nonlinear integral equation using Green's function. The nonlinear integral is written in an iterative form then solved numerically. The monotone solution needs initial guess. Convergence of the solution using the possible initial guesses including $u_0(x)=0$ and $u_0(x)=x/3$ were examined. The obtained results are compared with numerical ones. The results show, by using $u_0(x)=0$ in the monotone method, the solution for buckling of MWCNT cantilevers will be converge to numerical results with less iteration than using $u_0(x)=x/3$. As seen in figures and table 1, monotone solution after a few iterations almost converged to the numerical results. Furthermore, accuracy of monotone method is better than Adomian method. Therefore, the monotone iterative solution can provide an accurate and stable solution for study of MWCNT cantilevers.

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