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Buckling of multi wall carbon nanotube cantilevers in the vicinity of graphite sheets using monotone positive method

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Abstract

In this paper, a monotone positive solution is studied for buckling of a distributed model of multi walled carbon nanotube (MWCNT) cantilevers 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 based 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 the presented method, the results are compared with numerical results of a numerical method as well as other methods reported in the literature. The results show that the monotone iterative solution is stable and converged to numerical results with a few iterations. The results of the present work are useful to prove the stability and convergence of Green's function to deal with deflection of nano cantilever actuators in future works and simplifications.

Nomenclature

C_6	attractive constants for the carbon–carbon interaction	q_{Wdv}	Van der Waals force per unit length of MWCNT
d	interlayer distance between graphite layers	R_i	inner MWCNT radius
D	gap between MWCNT and the graphite surface	R_o	outer radius of MWCNT radius
E_{eff}	Young's modulus of MWCNT	R_W	mean value of MWCNT radius
f_n	non dimensional force	s	position of arbitrary concentrated load
G	response to arbitrary concentrated load	U	deflection of MWCNT
I	cross-sectional moment of inertia of MWCNT	u	non dimensional buckling
k_i , p_i	dummy coefficients	u_i	monotone solution after ith iteration
L	length of MWCNT	X	position along MWCNT
N	graphene layers	x	non dimensional position
n	power index	δ	Dirac delta function
N_W	number of walls of MWCNT	σ	graphene surface density

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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 were reported capable of nano manipulation and electrical detection which were actuated by electrostatic forces between the nanotubes [5]. Production of a low-friction, nanoscale, linear bearing from an individual MWCNT is reported by Poncharalet et al. [6]. Static mechanical deflection of cantilevered multi-wall carbon nanotubes has been implemented in a transmission electron microscope (TEM) [7], while double-clamped, suspended, single nanotube and nanowire have been used as high frequency resonators [8, 9]. Nanotube-based, electrically driven, torsional actuators have also been reported [10, 11]. These studies show the potential to construct nanoscale 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 layers. Appling the nano-scale continuum models is a reliable trend to simulate the deflection of MWCNT interacting with extremely large number of graphite atoms. In a very recent work Koochi et al. [17] utilized a hybrid continuum model to investigate the molecular force-induced buckling of the cantilever freestanding MWCNT probes/actuators suspended over graphite layers. They carried out a relation for buckling of MWCNT probes/actuators in the vicinity of thin and thick graphite layers for the first time. The governing equation of their distributed model leads to a forth order nonlinear differential equation. Because of the nonlinearity of the proposed equation, 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, i.e. the equation of MWCNTs [17], is the same as the non-dimensional governing differential equation of nano cantilever beams with rectangular cross section subject to Casimir effect with neglecting electrical forces [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, a number of investigators assumed the electrostatic and intermolecular forces uniform along the beam [19-23], and some others 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 based on Green's function and then some simplifications [17, 18, 24, 25], but they never attempt to solve obtained Green's function directly without 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 and nano-tubes cannot be categorized in any of the mentioned works (i.e. [28-36]).

Koochi et al. [17] and Ramezani et al. [24, 25] used Green's 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 based on Green's function is introduced and solved directly for the first time to obtain buckling of MWCNT cantilevers.The results are compared with numerical results as well as simplified Green's function method those reported by Koochi et al. [17] and with power series results which are reported by Noghrehabadi et al. [26].

2. Mathematical model

Figure 1 shows a scheme of a typical freestanding MWCNT near a surface consisting of N graphene layers, with interlayer distance d = 3.35Å. 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.

3. 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 >10 [22-23], the governing equation of a cantilever MWCNT can be defined as following boundary value differential equation [17]:

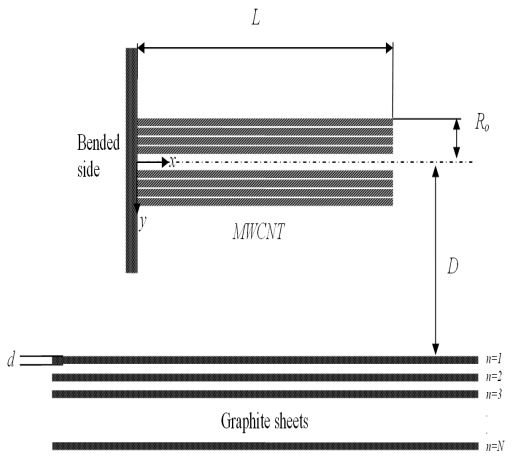


Fig. 1. Scheme of a MWCNT over graphite ground plane.

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

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

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

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

$$q_{wdv} = \begin{cases} \dfrac{C_6\sigma^2\pi^2 N_W R_W}{d\left(D-U\right)^4} & \text{For large number of layers} \\ \dfrac{4C_6\sigma^2\pi^2 NN_W R_W}{d\left(D-U+Nd/2\right)^4} & \text{For } small \text{ number of layers} \end{cases} \tag{2}$$

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

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

$$f_n = \begin{cases} \frac{C_6 \sigma^2 \pi^2 N_W R_W L^4}{d\ E_{eff}\ I\ D^5} & (n=4) \\ \frac{4 C_6 \sigma^2 \pi^2 N N_W R_W L^4}{E_{eff}\ I (D + Nd/2)^6} & (n=5) \end{cases} \tag{3}$$

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

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

$$u(0) = u'(0), at\ x=0,\ and\ u''(1) = u'''(1) = 0,\ at\ x=1 \tag{4-b}$$

where in all equations prime denotes differentiation with respect to x.

4. 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 Eq. (4-a) with $\delta(x - s)$, and by replacing the u with G in the left hand side, the following is obtained:

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

$$G(0) = G'(0) = 0, \quad at\ x=0$$
$$G''(1) = G'''(1) = 0, \quad at\ x=1 \tag{5-b}$$

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

$$G(x) = \begin{cases} k_0 x^3 + k_1 x^2 + k_2 x + k_3 & 0 \le x \le s \\ p_0 x^3 + p_1 x^2 + p_2 x + p_3 & s \le x \le 1 \end{cases} \tag{6}$$

The coefficients k_i and p_i in Eq. (6) are unknown constants. By imposing the boundary conditions at x=0 and x=1 the following equation is obtained:

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

Eq. (7) contains four unknown constants (k_0, k_1, p_2, p_3). These constants can be determined from remaining conditions. Three conditions come from continuity of nano-beam shape and its first and second derivatives at s;

$$G(s^-) = G(s^+),\ G'(s^-) = G'(s^+),\ G''(s^-) = G''(s^+) \tag{8}$$

The forth condition comes from integrating Eq. (5-a) across the point s to obtain the following:

$$G'''(s^+) - G'''(s^-) = 1 \tag{9}$$

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

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

Now, the derived Green's function is used to construct a solution to the uniform distributed

loading problem. Multiplying Eq. (5-a) by u and Eq. (4-a) by G, subtracting the two equations, and integrating from $x = 0$ to $x = 1$ leads to:

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

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

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

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

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

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, Eq. (4) will be solved by using Eq. (13) for f_n=0.5 and also for a range of f_n. The results of monotone solution are compared with numerical results.

5. Results and discussions

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

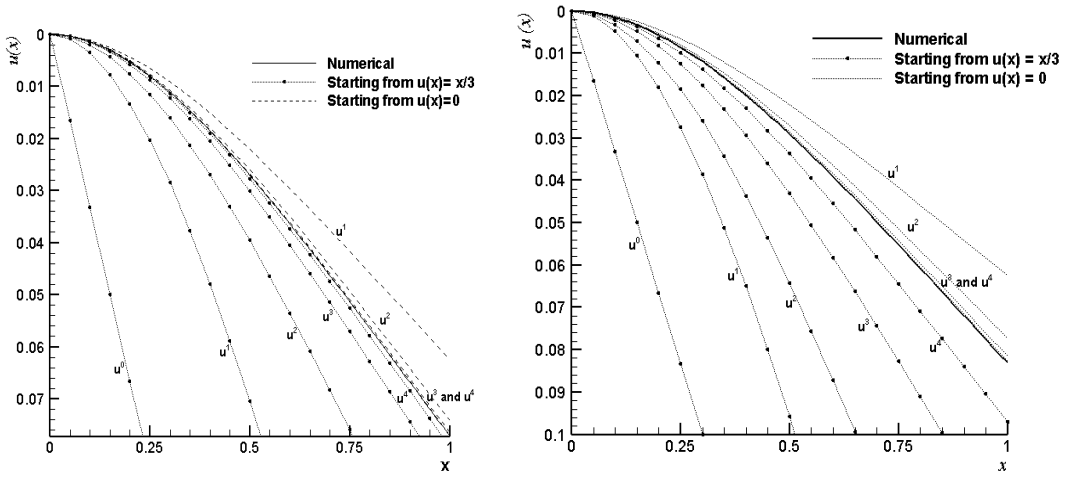
$$U^1(x) = \alpha\frac{x^2}{4} - \alpha\frac{x^3}{6} + \alpha\frac{x^4}{24} \tag{14}$$

Symbolic calculation of second and higher iterations of $u(x)$ is very complicated, and therefore, numerical integration is needed. In order to calculate integrals of Eq. (13) numerically, the adaptive Simpson quadrature integration method is used. In order to verify convergence and convergence rate of the monotone method, Eq. (4) solved with f_n=0.5 for small and large number of graphite layers which are used in the work of Koochi et al. [17]. Figs. (2a) and (2b) show the centerline deflection of a 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. It is clear that the monotone solution starting from $u_0(x)$ =0 overestimated the buckling of MWCNT cantilevers while the monotone solution starting from $u_0(x)$ =x/3 underestimated the buckling.

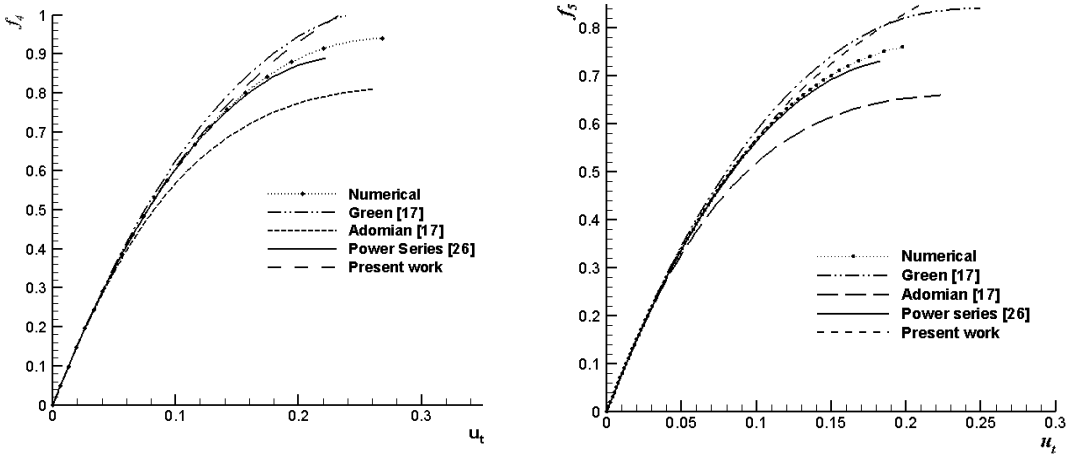
Table 1 compares the tip deflection of a nanotube cantilever obtained using monotone solution (by different starting values) with numerical results and Adomian series size of 10 which are obtained by Koochi et al. [17]. Numerical results are obtained using fifth order Runge–Kutta–Fehlberg scheme with shooting method [43].

Table 1 shows that the accuracy of monotone solution with starting from $u_0(x)$ =0 is more than that starting from $u_0(x)$ =x/3. Therefore, $u_0(x)$ =0 is chosen in later calculations. Figure 3 shows the variation of cantilever tip deflection as a function of f_n for large and small number of graphite layers. In this figure, the centerline buckling of nanotubes obtained by monotone method is compared with numerical results, Green, Adomian [17, 26], and series solution [26] methods for small and large number of graphite layers.



(a) **(b)**

Fig. 2. Buckling of MWCNT cantilever when f_n = 0.5 for to different iterations of monotone solutions and different starting values for : (a). with large number of graphite sheets (n = 4) and (b). small number of graphite sheets (n = 5).



(a) **(b)**

Fig. 3. Comparing the tip buckling of MWCNT cantilever obtained by monotone solution with $u_0(x)$ =0 and

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.

	n = 4			n = 5		
Iteration	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 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 numerical method
1	0.0625	0.0625	0.07719	0.0625	0.2813	0.083234
2	0.074073	0.074073		0.0773	0.1890	
3	0.076515	0.076515		0.0815	0.1251	
4	0.077044	0.077044		0.0827	0.0971	

6. Conclusions

In the present paper, a monotone positive solution is studied to obtain buckling of MWCNT cantilevers with small and large number of graphite layers subject to distributed Van der Waals attractions. The governing differential equation is forth order and nonlinear due to the inherent of the Van der Waals 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 as well as other methods. The findings of the present research can be summarized as follows:

-The monotone solution with both initial guesses, i.e. $u_0(x)$ = 0 and $u_0(x)$ = x/3, after a few iterations almost converged to the numerical results for comparatively small values of f_n.

-The monotone solution using $u_0(x)$=0 converged to the numerical solution with less iteration than using $u_0(x)$ = x/3.

-Comparison between the results of monotone method and the Adomian decomposition method show that the accuracy of monotone method is better than Adomian method.

-Comparison between the results of monotone solution and Green's function show that the accuracy of direct solution, i.e. monotone solution, is more than the Green's function.

-Based on the obtained results, the power series method is the most accurate method in this study, but it fails to capture a solution near the high values of dimensionless force f_n.

-Finally, the monotone iterative solution can provide an accurate and stable solution for study of MWCNT cantilevers.

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