Simulating the buckling deflection of carbon nanotube-made detectors used in medical detections by applying a continuum mechanics model

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Abstract: Carbon nanotubes are increasingly used in fabrication of nano-detectors and other nano devices. Herein, the buckling of a carbon nano-tube made detector is simulated. In order to obtain nonlinear constitutive equation of the detectors we assume the distributed electrostatic and Van der Waals attractions along the CNT length. By considering the nano forces in a continuum mechanics model we were able to achieve the differential equation of the CNT. In the next step by applying Adomian series solution, we provided an analytical closed-form solution of CNTs. The deflection and the buckling parameters are determined and discussed in detail. The analytical obtained results are compared with those of literature as well as numerical solution. The obtained results revealed that the presented continuum based model is in good agreement with experimental result. Moreover it is found that the analytical solution can be considered as a reliable approach to study the buckling stability of detectors in nanoscales where the presence of van der Waals force is important.
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Key words: Carbon nanotube (CNT), Buckling, Continuum model, Nano-detector, Electrostatic, Modified Adomian method (MAD).

1. Introduction

After discovering carbons nano-tubes (CNTs), these materials are increasingly used in manufacturing small-scale structures. In recent decades these materials are specially for constructing nano-detectors, nanotweezers, nanoelectromechanical switches, etc. (Paradise *et al.,* 2007; Baughman *et al.,* 1999; Ke *et al.,* 2005). It has been demonstrated that the elastic modulus, bending flexibility and tensile strength of carbon nano-tubes are much higher than the conventional metallic materials (Esawi and Farag, 2007). These materials have a great potential for medical applications in manufacturing medical detectors, biological sensors etc. Assume a typical cantilever CNT detector suspended near electrode surface with a small gap in between. By applying a voltage difference between the nano-components causes the CNT to deflect and be attracted toward the electrode surface due to the presence of electrostatic forces. Once this voltage exceeds a critical value, an increase in the electrostatic force becomes greater than the corresponding increase in the restoring force, resulting in the unstable collapsing of the CNT to the ground position. This behavior is known as the buckling instability and the critical voltage is called the buckling voltage. Predicting this voltage is very important for engineers.

While there are several forces such as casimir, capillary and van der Waals force that are acting in sub-micro distances. As the gap decreases from micro to nano-scale, the van der Waals interaction occurs. The prediction of the molecular force-induced instability of CNTs nano-detector is a critical subject in design nano-detector: A nano-detector might adhere to its substrate with an applied voltage less than buckling voltage or even without an applied voltage as a result of molecular force, if the minimum gap between the nano-detector and substrate is not considered (Lin and Zhao, 2005;Abadyan *et al.,* 2010;Koochi *et al.,* 2011; Tsai and Tu, 2010; Tserpes, 2007; Desquenes *et al.,* 2002; Batra and Sears, 2007; Lin and Zhao, 2005; Hayt and Buck, 2001). Therefore predicting the effect of nano-scale forces on performance of the nano-detector is very important issue for design reliable detectors.

There are several approaches for investigate the nano-world. In order to simulate the nanomaterials, several theoretical techniques might be employed by researchers. The most famous molecular dynamics (MD) and molecular mechanics (MM) simulations could be used to study the mechanical behavior of carbon-based nano-materials (Tsai and Tu, 2010; Tserpes, 2007; Desquenes *et al.,* 2002; Batra and Sears,2007). However these methods are very time-consuming and might not be easily used in complex structures.

Although continuum models are more time-saving than MM and MD, their approach often leads to nonlinear equations that might not be worked out by analytical methods, accurately (Desquenes *et al.,* 2002; Lin and Zhao, 2005). Therefore analytical approaches are used to solve the constitutive equations of the nano-system.

Due to the importance of the instability of CNT nano-detectors this work is dedicated to simulating the instability of the nano-detectors. In this paper, the buckling instability of cantilever CNT detector has been studied. Modified Adomian decomposition (MAD) is employed to solve the nonlinear governing equation of the system. The obtained results are verified by comparing with those from literature as well as numerical solution. Results will be useful for design the nano-detectors.

2. Theoretical Model

2.1. Electrostatic interaction

Let us consider a freestanding multi-walled CNT above a ground plane consisted of graphene layers, with interlayer distance d = 3.35 Å, as illustrated in Fig. 1. When a conductive nano-tube is placed over an electrode substrate in the presence of an applied potential difference between the tube and the electrode, the electrostatic charge would be induced both on the tube and the substrate. To calculate the electrical forces acting on the tube, a capacitance model may be used. For infinitely long metallic cylinders, the capacitance per unit length is given by (Hayt and Buck, 2001):

$$C(q) = \frac{2\pi\varepsilon_0}{\operatorname{arccosh}(1+\frac{D}{R_w})} \qquad (1)$$

Where D is the initial distance between the tube and ground plate, ε_0=8.854×10^{-12} C^2/Nm^2 is the permittivity of vacuum so the electrostatic force per unit length is given by:

$$f_{elec} = \frac{d(\frac{1}{2}C(D)V^2)}{d(D)} = \frac{\pi\varepsilon_0 V^2}{\sqrt{D(D+2R_w)}\operatorname{arccosh}^2(1+\frac{D}{R_w})} \qquad (2)$$

Where R_w the radius of CNT and V the applied voltage.

By applying external voltage the nano-tube deflected to ground and the distance between the nano-tube and ground plate reduce to D-U therefore the electrostatic force per unit length of deflected detector can be rewrite as:

$$f_{elec} = \frac{\pi\varepsilon_0 V^2}{(D-U)\operatorname{arccosh}^2(\frac{D-U}{R_W})} \qquad (3)$$

It's must be noted in this equation we assumed that:

$$D \pm R_w \approx D \qquad (4)$$

Equation (3) can be simplified by using the following assumption:

$$\frac{1}{(D-U)\operatorname{arccosh}^2(\frac{D-U}{R_W})} = \frac{1}{D-U}\left(\frac{1}{\ln[(\frac{D-U}{R_W})+\sqrt{(\frac{D-U}{R_W})^2-1}]}\right)^2 \approx \qquad (5)$$

$$\frac{1}{D-U}\times\frac{1}{\ln^2[2\frac{D-U}{R_W}]}$$

Therefore

$$f_{elec} = \frac{\pi\varepsilon_0 V^2}{(D-U)\ln^2(2\frac{D-U}{R_W})} \qquad (6)$$

2.2. van der Waals interactions

Lennard-Jones potential is a suitable model to describe van der Waals interaction (Lennard-Jones, 1930). It defines the potential between atoms i and j by

$$\varphi_{ij} = \frac{C_{12}}{r_{ij}^{12}} - \frac{C_6}{r_{ij}^6} \qquad (7)$$

whre r_{ij} is the distance between atoms i and j while C_6 and C_{12} are the attractive and repulsive constants, respectively. For distances higher than 3.4 Å, such as in this paper, the repulsive term decays extremely fast and can be neglected (Tserpes, 2007). For the carbon-carbon interaction, C_6=15.2 eVÅ^6 (Girifalco *et al.,* 2000). A reliable continuum model has been established to compute the van der Waals energy by double-volume integral of Lennard-Jones potential (Ke and Espinosa, 2006), that is

$$E_{vdW} = \int_{\upsilon_1}\int_{\upsilon_2} n_1 n_2 \left(-\frac{C_6}{r^6(\upsilon_1,\upsilon_2)}\right) d\upsilon_1 d\upsilon_2 \qquad (8)$$

where υ_1 and υ_2 represent the two domains of integration, and n_1 and n_2 are the densities of atoms in these domains, respectively.

The distance between any two points on υ_1 and υ_2 is $r(\upsilon_1,\upsilon_2)$.

Eq. (8) provides acceptable results for explaining the CNT-graphene attraction compared to that of direct pair wise summation through molecular dynamics in Eq. (7). For a (15,0) single walled carbon nanotube (SWCNT) over a graphene surface and for distances larger than 5 Å, the difference between E_{vdW} specified by Eq. (8) and molecular dynamics, is less than 1% (Tserpes, 2007).

Let us consider a freestanding multi-walled CNT above a ground plane consisted of graphene layers, with interlayer distance d = 3.35 Å, as illustrated in Fig. 1. The length of CNT is L and the initial gap between CNT and the ground is D. The boundary condition of the CNT is defined as cantilever at one end (with no displacement and rotation) and traction free at the free end (with no shear force and moment).

Using Eq. (8), the energy per unit length of nano-tube is simplified to (Tserpes, 2007):

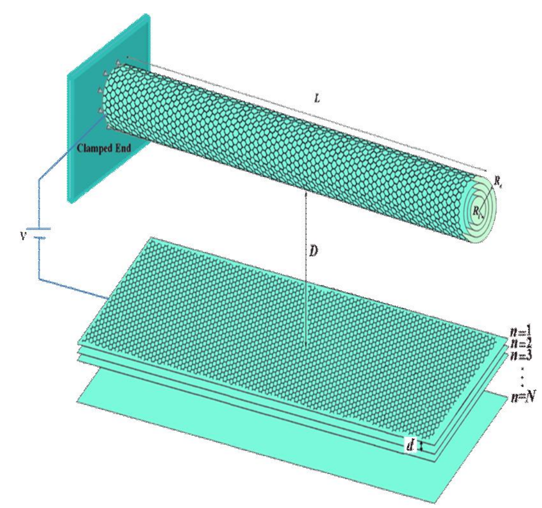


Figure1. Schematic representation of Cantilever CNT nano-detector

$$\frac{E_{vdW}}{L}=-C_6\sigma^2\pi^2\sum_{R=R_i}^{R_o}\sum_{r=D}^{D+(N-1)d}\frac{R(R+r)[3R^2+2(R+r)^2]}{2[(R+r)^2-R^2]^{3.5}} \tag{9}$$

where R_i and R_o are the inner and outer radii of CNT, N is the number of graphene sheets and $\sigma \cong 38\text{nm}^{-2}$ is the graphene surface density. Once the van der Waals energy is computed, the corresponding energy terms are employed to derive the component of the intermolecular force per unit length, f_{vdW}, along r-direction as below:

$$f_{vdW}=-\frac{d(\frac{E_{vdW}}{L})}{dr}= C_6\sigma^2\pi^2\sum_{R=R_i}^{R_o}\sum_{r=D}^{D+(N-1)d}\frac{R(8r^4+32r^3R+72r^2R^2+80rR^3+35R^4)}{2r^{4.5}(r+2R)^{4.5}} \tag{10}$$

In most applications it is practically assumed that the diameter of tubes is much smaller than the distance between nanotube and the graphene surface, i.e. $(2R)<<D$. According to this assumption, Eq. (10) is simplified to

$$f_{vdW}(r)=4C_6\sigma^2\pi^2N_WR_W\sum_{r=D}^{D+(N-1)d}\frac{1}{r^5} \tag{11}$$

where N_W is the number of walls of nanotube and R_W is the mean value of their radii.

For large number of layers, i.e. $D+(N-1)d >> D$, substitution of the summation with an integral results:

$$\sum_{r=D}^{D+(N-1)d}\frac{1}{r^5}\approx\frac{1}{d}\int_D^{D+(N-1)d}\frac{1}{r^5}dr =\frac{1}{4d}\left[\frac{1}{D^4}-\frac{1}{(D+(N-1)d)^4}\right]\approx\frac{1}{4dD^4} \tag{12}$$

Lastly we have:

$$f_{vdW}(D)\approx C_6\sigma^2\pi^2N_WR_Wd^{-1}D^{-4} \tag{13}$$

2.3. Governing equations

In order to develop the governing equation of the beams, the constitutive material of the nano-tube is assumed to be linear elastic, and only the static deflection of the nano-tube is considered. The minimum energy principle was applied, which implies equilibrium when the free energy reaches a minimum value. By applied the Hamilton principle the governing equilibrium equation can be determined as:

$$\begin{aligned}\delta W &= \delta W_{elas}-\delta W_{elec}-\delta W_{vdW}\\ &=\int_0^L\left(E_{eff}I\frac{d^2U}{dX^2}\delta\frac{d^2U}{dX^2}-f_{elec}\delta U-f_{vdW}\delta U\right)dX\\ &=E_{eff}I\frac{d^2U}{dX^2}\delta\frac{dU}{dX}\Big|_0^L-E_{eff}I\frac{d^3U}{dX^3}\delta U\Big|_0^L\\ &+\int_0^L\left(E_{eff}I\frac{d^4U}{dX^4}-f_{elec}-f_{vdW}\right)\delta U dX=0\end{aligned} \tag{14}$$

Where δ denotes the variation symbol, X is the position along the nano-tube measured from the clamped end, U is the beam deflection, E_{eff}, is the effective Young's modulus of CNT which is typically 0.9-1.2 TPa (Gupta and Batra, 2008) and I is the cross-sectional moment of inertia, equal to $\pi(R_o^4 - R_i^4)/4$.

By integrating Eq.(14), the governing equation of cantilever nano-tube detector is derived as:

$$EI\frac{d^4U}{dX^4} = f_{elec} + f_{vdW} \qquad (15.a)$$

With the B.C. of:

$$U(0) = \frac{dU}{dX}(0) = 0$$

(Geometrical B.C. at fixed end), (15.b)

and

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

(Natural B.C. at free end). (15.c)

Eqs. (15a-c) can be made dimensionless using the following substitutions,

$$u = \frac{U}{D},$$

$$x = \frac{X}{L},$$

$$\alpha = \frac{C_6\sigma^2\pi^2 N_W L^4}{dE_{eff} ID^4}, \qquad (16)$$

$$\lambda = \frac{D}{R_W},$$

$$\beta = \frac{\pi\varepsilon_0 V^2 L^4}{E_{eff} ID^2}$$

These transformations yield

$$\frac{d^4u}{dx^4} = \frac{\alpha}{\lambda(1-u(x))^4} + \frac{\beta}{(1-u)\ln^2[2\lambda(1-u)]} \qquad (17\text{-a})$$

With the B.C. :

$$u(0) = \frac{du}{dX}(0) = 0 \qquad (17\text{-b})$$

(Geometrical B.C. at fixed end),

and

$$\frac{d^2u}{dx^2}(L) = \frac{d^3u}{dx^3}(L) = 0 \qquad (17\text{-c})$$

(Natural B.C. at free end).

3. Solution

In this section two solving methods has been applied for solving the governing equation. First is MAD and the second is Nemerical solution:

3.1 Adomian series solution

The detail of the MAD can be find in (Adomian, 1983). The analytical MAD solution of equation (17) can be obtained as the following:

$$\begin{aligned}
u(x) = & -\frac{1}{2!}C_1x^2 - \frac{1}{3!}C_2x^3 + \frac{1}{4!}\left(\frac{\alpha}{\lambda} + \frac{\beta}{\ln^2(2\lambda)}\right)x^4 \\
& -\frac{1}{6!}\left(\frac{4\alpha}{\lambda} + \frac{\beta}{\ln^2(2\lambda)} + \frac{2\beta}{\ln^3(2\lambda)}\right)C_1x^6 \\
& -\frac{1}{7!}\left(\frac{4\alpha}{\lambda} + \frac{\beta}{\ln^2(2\lambda)} + \frac{2\beta}{\ln^3(2\lambda)}\right)C_2x^7 \\
& +\frac{1}{8!}\{\left(\frac{\alpha}{\lambda} + \frac{\beta}{\ln^2(2\lambda)}\right)\left(\frac{4\alpha}{\lambda} + \frac{\beta}{\ln^2(2\lambda)} + \frac{2\beta}{\ln^3(2\lambda)}\right)C_2 \\
& +\left[\frac{60\alpha}{\lambda} + \frac{6\beta}{\ln^2(2\lambda)}\left(1 + \frac{3}{\ln(2\lambda)} + \frac{3}{\ln^2(2\lambda)}\right)\right]C_1\}x^8 \\
& +\frac{1}{9!}\left[\frac{200\alpha}{\lambda} + \frac{20\beta}{\ln^2(2\lambda)}\left(1 + \frac{3}{\ln(2\lambda)} + \frac{3}{\ln^2(2\lambda)}\right)\right]C_1C_2x^9 \\
& +\ldots
\end{aligned} \qquad (18)$$

Where the constants C_1 and C_2 can be determined by solving the resulting algebraic equation from the B.C at $x=1$ i.e. using equation (17-c).

For any given α, β and λ, equation (31) can be used to obtain the buckling parameters of the nano-tube detector. The instability in equation (18) occurs when $d\beta(x=1)/du \rightarrow 0$. The buckling voltage of the system can be determined via plotting the u vs. β.

3.2 Numerical Solution

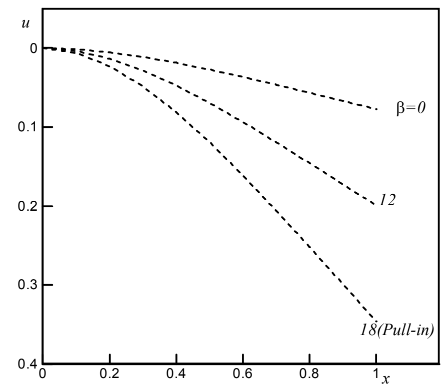
In order to verify the analytical results, the cantilever beam-type nano-detector is numerically simulated and the results are compared with those obtained via MAD and LPM. The nonlinear governing differential equation (Eq. (17)) is solved with the boundary value problem solver of MAPLE commercial software. The step size of the parameter variation is chosen based on the sensitivity of the parameter to the tip deflection. The buckling parameters of the system can be determined via the slope of the u-β graphs.

4. Results and Discussion

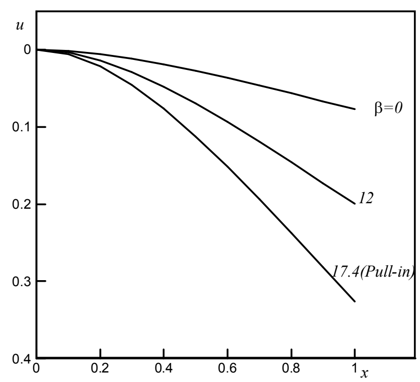
4.1. Verification

First we verify the solution with experiments. In order to verify the obtained results, the buckling voltage of a typical cantilever CNT base nano-detector with the following parameters was compared to experimental data in Table. 1. The length of the nanotube, L= 6:8 µm; initial gap between nanotube and electrode, D = 3 µm; R_w=5nm; E = 1 TPa. As seen the MAD results are in good agreement with experimental results.

4.2. Simulation of deflection



(a)



(b)

Figure 2. Deflection of the cantilever CNT for different values of β when α=25 and λ=10. (a) analytical, (b) Numerical

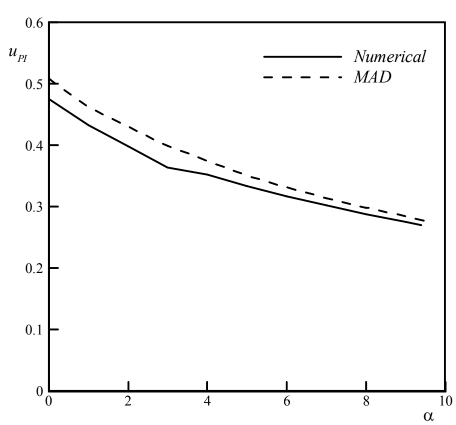


Figure 3. Effect of van der Waals force (f) on pull-in deflection (λ=10)

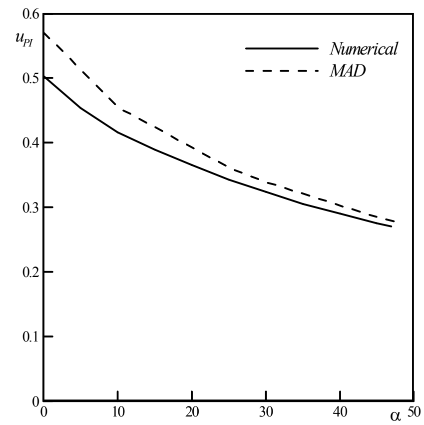


Figure 4. Effect of van der Waals force (f) on pull-in deflection (λ=50)

After validating the solution by experiments, we simulate the deflection of the nano-detector. Figure 2 shows the centerline deflection of a typical nano-tube detector under intermolecular force and external voltage obtained using MAD, and numerical methods. This figure u_{tip} increases from zero to u_{tip}^*, when α increases from zero to α^*. This figure reveals that the CNT nano-detector has initial deflection without applying voltage difference. This is the result of the presence of vdW attraction.

4.3 Effect of van der Waals force on deflection of CNT

The buckling deflection is an important parameter for design the detectors. The relation between buckling deflection and van der Waals force (α) is presented if figure 3 and 4 for 2 different values of *radios* to initial gap ratio (λ=10 and λ=50) as seen increasing the intermolecular force the buckling voltage decrease. When no voltage applied (β=0) the CNT buckling if the van der Waals force exceeds from its critical values (α^*) the critical values of α can find from the horizontal axes of figure 3 and 4. By comparing Figure 3 and 4 reveal that by increasing the values of λ, the critical values of α increase as well as the buckling voltage.

Table 1. Buckling voltage obtained from different method

Method	Experimental (Ke *et al.*,2005)	MAD	Numerical
Buckling Voltage	48	50.39	48.79

5. Conclusions

The buckling behavior of a cantilever CNT nano-detector has been studied. The obtained results show that:

The Adomian series solution is a very power full method for study the buckling behavior of CNT based nano-detectors.

In the absence of electrical loading on CNT based detector, it can buckling to ground if the van der Waals force exceeds from its critical values and this critical values increase if the λ increase.

The van der Waals force reduces the instability deflection of the CNT detector.

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