MODELING THE STABILITY OF FREESTANDING CNT PROBE/SENSOR IN THE VICINITY OF GRAPHENE LAYERS CONSIDERING CASIMIR DISPERSION FORCE

Rouhollah Shokuhifard[1], Mojtaba Ojakeh[2], Ameneh Langari[3] and Maryam K. Hafshejani[4]
[1]Department of Physics, Andimeshk Branch, Islamic Azad University, Andimeshk, Iran
[2]Physics group, Department of Science, Dezful Branch, Islamic Azad University, Dezful, Iran
[3]Bojnurd University of Medical Sciences, Bojnurd, Iran
[4]Shahrekord University of Medical Sciences, Shahrekord, Iran
E-Mail: maryam.keivani@yahoo.com

ABSTRACT

Carbon nanotube (CNT) is one the most important nano-elements in fabrication of probes, sensors and other ultra-small devices that have a wide usage in engineering and medicine. In this paper, the deflection and instability of a freestanding CNT probe/sensor in the vicinity of the graphene layers are investigated. A nano-scale continuum model in conjunction with Euler beam theory is employed to obtain nonlinear constitutive equation of freestanding CNT by considering the effect of Casimir dispersion force. A numerical finite difference method is employed to solve the nonlinear governing equation.

Keywords: carbon nanotube (CNT), graphene layers, deflection, instability, nano-scale continuum model, casimir force.

INTRODUCTION

Recently, carbon nanotubes (CNTs) have become the center of interest for many scientists due to their large application such as microscope probes/sensors (Jeong *et al*., 2006; Lim *et al*., 2007; Mann *et al*., 2006) and actuators/switches (Desquenes *et al*., 2002; Hwang and Kang, 2005; Ke *et al*., 2005). Figure-1 depicts a schematic CNT-based probe/sensor constructed from a freestanding nanotube which is suspended from a clamped end near graphene ground with small gap between CNT and the ground. With the decrease in dimensions from micro to nano-scale, CNT deflects to the substrate due to the Casimir interaction between CNT and graphene sheets. Especially, when the separation is small enough, the nanotube becomes unstable and buckles onto the graphene layers. The maximum length of CNT that does not stick to the ground plane is called the stable length. In other words, the stable length is the maximum permissible length of freestanding CNT. Alternatively, for a known CNT length, there is a minimum initial gap between CNT and the substrate to ensure that CNT does not adhere to the substrate by dispersion force. Determination of stable length and minimum gap of freestanding nanostructures is important in designing and manufacturing nano-probes and nano-switches (Snow *et al*., 2002a; 2002b; Lin and Zhao, 2003; 2005a; 2005b; Wang *et al*., 2004; Zhao *et al*., 2003).

In order to investigate the mechanical behavior of CNT, several approaches are employed. Molecular mechanics simulation may be used to study the CNT/grapheme interaction an alternative reliable approach to nano-scale simulation is applying nano-scale continuum models (Desquenes *et al*., 2002; Ke *et al*., 2005; Koochi *et al*., 2011a; Strus *et al*., 2008).

In this paper, we have investigated the deflection and instability of a cantilever freestanding CNT suspended near graphene layers. Finite difference method is employed to solve constitutive equation of the probe/sensor. In addition, the minimum gap and the permissible length of CNT that does not stick to graphene layers due to Casimir attraction are computed as functions of geometrical and material characteristics.

GOVERNING EQUATION

In order to develop the governing equation of the CNT, the constitutive material of the nanotube is assumed to be linear elastic, and only the static deflection of the nanotube is considered. The elastic potential energy and the work done by molecular and electrical forces can be expressed as:

$$U_{elas} = \frac{1}{2}\int_0^L E_{eff} I \left[\frac{d^2u}{dX^2}\right]^2 dX \quad 1(a)$$

$$W_{Cas} = \int_0^L\int_0^u f_{Cas}\, du dX \quad 1(b)$$

where U_{elas}, and W_{Ca} are the elastic energy and the work done by molecular force, respectively. By applying minimum energy principle, i.e., $\delta(U\text{-}W) = 0$, the following equation is obtained:

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$$\begin{aligned}\delta W &= \delta U_{elas} - \delta W_{Cas}\\ &= \int_0^L (E_{eff} I \frac{d^2\hat{u}}{dX^2}\delta\frac{d^2\hat{u}}{dX^2} - f_{Cas}\delta\hat{u})dX\\ &= E_{eff} I \frac{d^2\hat{u}}{dX^2}\delta\frac{d\hat{u}}{dX}\bigg|_0^L - E_{eff} I \frac{d^3\hat{u}}{dX^3}\delta\hat{u}\bigg|_0^L\\ &+\int_0^L (E_{eff} I \frac{d^4\hat{u}}{dX^4} - f_{Cas})\delta\hat{u}dX = 0,\end{aligned} \tag{2}$$

Where δ denotes the variation symbol, X is the position along the nano-tube measured from the clamped end, $\hat{u}$ is the CNT deflection, E_{eff} is the effective Young's modulus of the CNT, which is typically 0.9-1.2 TPa (Koochi *et al*., 2011b) and I is the cross-sectional moment of inertia. By integrating Equation (2), the governing equation of the cantilever nano-tube probe is derived as:

$$E_{eff} I \frac{d^4 u}{dX^4} = f_{Cas}, \qquad 3(a)$$

$$\hat{u}(0) = \frac{d\hat{u}}{dX}(0) = 0 \text{ (Geometrical B.C. at the fixed end)} \qquad 3(b)$$

$$\frac{d^2\hat{u}}{dX^2}(L) = \frac{d^3\hat{u}}{dX^3}(L) = 0 \text{ (Natural B.C. at the free end)} \qquad 3(c)$$

Where f_{Cas} is the casimire force between a cylinder and plate which can explain as (Kenneth *et al*., 2002; Bordag *et al*., 2001):

$$f_{Cas} = \frac{1}{768}\pi^3\hbar c\sqrt{\frac{2R}{(g-\hat{u})^7}} \tag{4}$$

Where R is the radius of CNT, g is the initial gap between the movable and the ground electrode, $h = 1.055\times10^{-34}$ Js is Planck's constant divided by 2π and $c = 2.998\times10^8$ m/s is the light speed.

Equations 4(a-c) can be made dimensionless using the following substitutions:

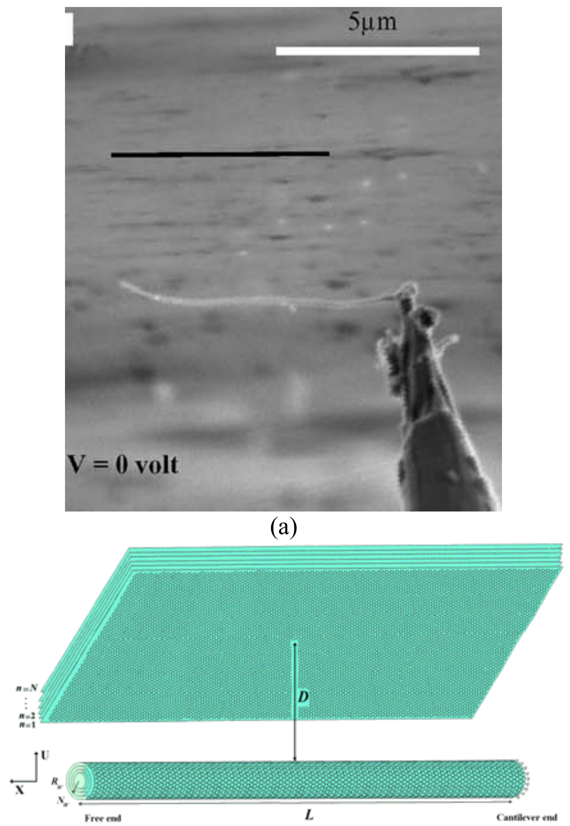
$$\begin{aligned} u &= \frac{\hat{u}}{g},\\ x &= \frac{X}{L},\\ f &= \frac{\text{h}c\pi^3 L^4\sqrt{2R}}{768E_{eff} I g^{4.5}}.\end{aligned} \tag{5}$$

These transformations yield

$$\frac{d^4 u}{dx^4} = \frac{f}{(1-u(x))^{3.5}}, \qquad 6(a)$$

$$u(0) = \frac{du}{dx}(0) = 0 \text{ (Geometrical B.C. at the fixed end),} \qquad 6(b)$$

$$\frac{d^2 u}{dx^2}(1) = \frac{d^3 u}{dx^3}(1) = 0 \text{ (Natural B.C. at the free end)} \qquad 6(c)$$



(a)

(b)

Figure-1. a) SEM images of a freestanding CNT probe (Ke *et al*., 2005) and b) its schematic continuum model.

SOLUTION

In order to solve the nonlinear governing equation, a procedure based on finite difference method (FDM) is developed in this study for making meaningful comparisons. Following the standard FDM procedure, the beam is discretized into n equal sections (elements) separated by (n + 1) nodes. For each element, the governing equation (6) in the discretized form can be written as:

$$\frac{u_{i-2} - 4u_{i-1} + 6u_i - 4u_{i+1} + u_{i+2}}{\Delta x^4} = F_i \tag{7}$$

where Δx is the grid spacing, u_i is the deflection of i^{th} grid and:

$$F_i = \frac{f}{(1-u_i)^{3.5}} \tag{8}$$

Applying equation (7) to all of the elements and incorporating the boundary conditions (equation 6(b) and 6(c)), a matrix form equation is obtained as:

$$[A]\{w\} = \{F\} \tag{9}$$

Where $\{w\} = [w_1, w_2, ..., w_n]^T$, $\{F\} = [F_1, F_2, ..., F_n]^T$ and A matrix can be defined as:

$$[A] = \begin{bmatrix} 7 & -4 & 1 & 0 & 0 & \dots & 0 & 0 & 0 & 0 \\ -4 & 6 & -4 & 1 & 0 & \dots & 0 & 0 & 0 & 0 \\ 1 & -4 & 6 & -4 & 1 & \dots & 0 & 0 & 0 & 0 \\ 0 & 1 & -4 & 6 & -4 & \dots & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & -4 & 6 & \dots & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & -4 & \dots & 0 & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & 0 & \cdots & -4 & 6 & -4 & 1 \\ 0 & 0 & 0 & 0 & 0 & \cdots & 1 & -4 & 5 & -2 \\ 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 1 & -2 & 1 \end{bmatrix} \tag{10}$$

Matlab commercial software is employed to numerically solve equation (10) for the nodal deflections that govern the overall deflection of the beam.

RESULTS AND DISCUSSIONS

The FDM solution can be employed to investigate the instability of CNT. For any given f, where $f \le f^*$, there are a solution for u. When $f > f^*$, no solution exists for u_{tip}. This means that CNT collapses onto the graphene ground.

Figure-2 shows the centerline deflection of a typical CNT probe/actuator for different Caimir force from zero to critical value. As seen by increasing the Casimir force the deflection of CNT increase and in the critical values of Casimir force the beam has the maximum deflection.

The relations between Casimir (f) and the free-end deflection of a typical CNT (u_{tip}) are presented in Figure-3. When f exceeds the critical value f^*, no solution exists for u_{tip} and the buckling occurs.

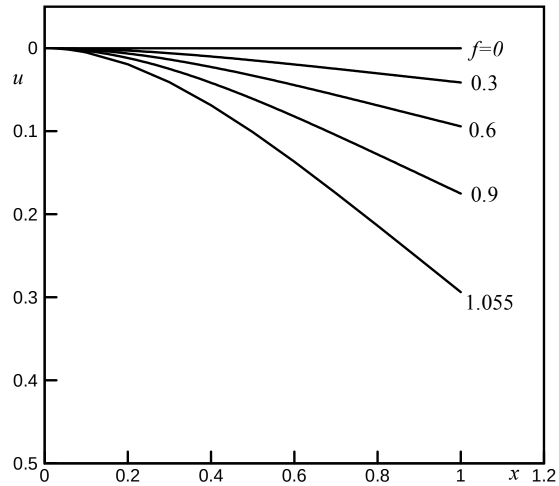


Figure-2. Deflection of the cantilever CNT for different values of f from zero to critical values.

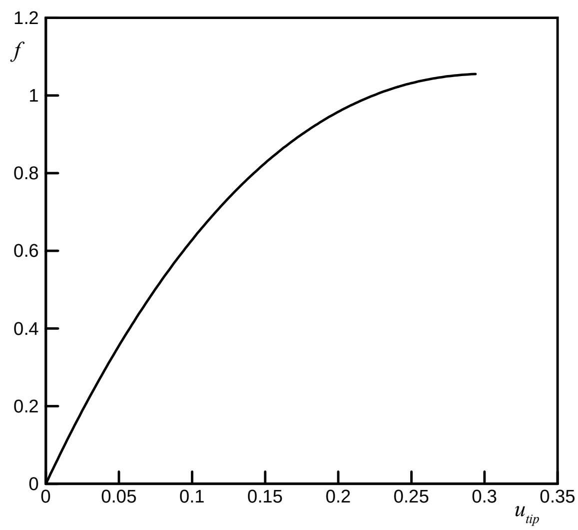


Figure-3. Relationship between f and the CNT tip deflection Collapse occurs when f reaches values greater than f^*.

As mentioned earlier, the stable length, L_{max}, is the maximum length of CNT that does not stick to graphene substrate due to Casimir force. The stable length is an important parameter for engineering applications such as CNT-based nano-switches or probes design. Substituting f^* into definition of f in Equation (5), L_{max} is gained. As an alternative case, if the length of CNT is known, then one can calculate the minimum gap, g_{min}, between CNT and the substrate to ensure that nanotube does not adhere to the graphene ground.

$$L_{max} = \sqrt[8]{\frac{294912 f^{*2} E_{eff}^{\ 2} I^2 g^9}{\mathrm{h}^2 c^2 \pi^6 R}} \tag{11}$$

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$$g_{\min} = \sqrt[9]{\frac{\mathrm{h}^2 c^2 \pi^6 L^8 R}{294912 E_{eff}^2 I^2 f^{*2}}}. \tag{12}$$

For our FDM solution;

$$L_{max} = 4.892 \sqrt[8]{\frac{E_{eff}{}^2 I^2 g^9}{\mathrm{h}^2 c^2 \pi^6 R}} \tag{13}$$

$$g_{\min} = 0.244 \sqrt[9]{\frac{\mathrm{h}^2 c^2 \pi^6 L^8 R}{E_{eff}^2 I^2 f^{*2}}}. \tag{14}$$

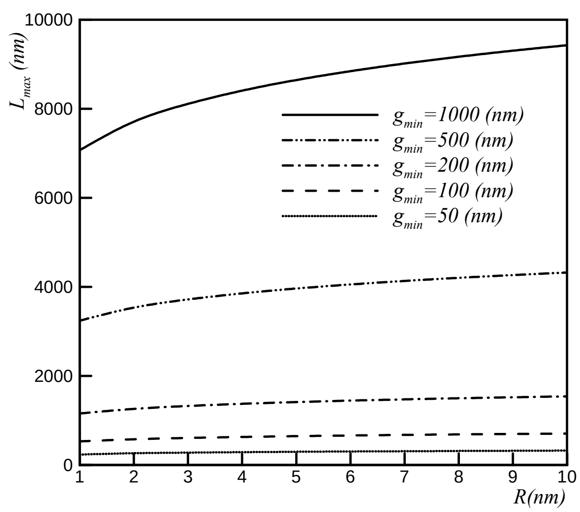

Figure-4. Detachment length of the single walled CNT as a function of the nanotube radius for various minimum gaps.

As a case study, a cantilever single walled CNT with Young's modulus of 1 TPa is considered. In this case, I is approximately $\pi t R_W{}^3$, where t is the thickness of CNT, typically about 0.35 nm (Koochi *et al*., 2011b). Figure-4 depicts the variation of CNT stable length as a function of the nanotube diameter and initial gap.

Finally, note that the physics of CNT/ground attraction is a non-linear phenomenon and the solution is valid for small deformation instability behavior (Sasaki *et al*., 2006). In cases such as peeling CNT from graphite substrate or the case where the gap is of the order of CNT diameter, etc., large deflection of the nanotube should be considered in the formulas. Therefore, the present simple model must be modified or molecular mechanics should be applied alternatively to obtain more precise results (Sasaki *et al*., 2006).

CONCLUSIONS

In this paper, deflection and instability of CNT near the graphene layers has been studied using a nano-scale continuum model. Results indicate that Casimir force can collapse cantilever CNT at submicron. The proposed model is capable of predicting the critical values of Casimir force and CNT deflection at the onset of buckling. In addition, the stable length of CNT has been determined which is a fundamental design parameter in constructing CNT-based probes and switches. It is found that the stable length of CNT highly depends on geometrical dimensions of CNT such as radius.

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