Buckling of Multi Walled Carbon Nanotube Probes with Small Number of Layers near Graphite Sheets

Alireza Yekrangi*, Elyas Mohammadian

Mechanics group, Ramsar Branch, Islamic Azad University, Ramsar Iran
Email: Yekrangi_ali@yahoo.com

Abstract: Herein, deflection and instability of a freestanding carbon nanotube (CNT) probe/sensor in the vicinity of the graphene layers are investigated. Modeling the buckling of multi walled carbon nanotube (MWCNT) probes/actuators with small number of layers in the vicinity of thin and thick graphite has been carried out using numerical finite difference method. A hybrid nano-scale continuum model based on Lennard-Jones potential is applied to simulate the intermolecular force-induced deflection of MWCNT. The deflection of freestanding MWCNT near graphen plate and critical values of MWCNT tip deflection and MWCNT-graphite attraction at the onset of the instability are computed.
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1. Introduction

Carbon nanotubes (CNTs) have become the center of interest for many scientists due to their large application such as microscope probes/sensors and actuators/switches (Desquenes *et al.,* 2002; Hwang and Kang 2005; Ke *et al.,* 2005a). The extraordinary properties of MWCNTs have motivated engineers worldwide to explore their applications in different fields. With recent growth in nanotechnology, MWCNTs are increasingly used in developing atomic force microscope (AFM) probes (Li *et al.,* 2008; Akita 2001; Cao *et al.,* 2005) and nano-electromechanical system (NEMS) switches (Baughman *et al.,* 1999; Ke *et al.,* 2005a; Snow *et al.,* 2002). Consider a typical cantilever MWCNT probe/switch a shown if figure 1. 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. The prediction of the molecular force-induced instability of MWCNTs near the surface is a critical subject in design AFM probes and NEMS switches. With decrease in distance between the AFM probe and sample surfaces, the probe jumps into contact with the surfaces and renders its imaging performance (Snow *et al.,* 2002; Jalili *et al.,* 2004; Snow *et al.,* 2002). Similarly, a NEMS switch might adhere to its substrate even without an applied voltage as a result of molecular force, if the minimum gap between the switch and substrate is not considered (Abadyan *et al.,* 2010; Abdi *et al.,* 2011; Koochi *et al.,* ; 2010; 2011a; 2012; Soroush et al., 2010; Tadi Beni *et al.,* 2011a; 2011b).

In order to study nanomaterials, several approaches are employed. Molecular dynamics (MD) and molecular mechanics (MM) simulations could be used to study the mechanical behavior of carbon-based nanomaterials (Tsai and Tu 2010; Tserpes, 2007; Desquenes *et al.,* 2002; Batra *et al.,* 2007). However these methods are very time-consuming and might not be easily used in complex structures. An alternative reliable trend to simulate the instability behavior of MWCNT interacting with extremely small number of graphite atoms is to apply nano-scale continuum models. A hybrid continuum model can be used to calculate the van der Waals energy, in lieu of the discrete Lennard-Jones potential, similarly (Desquenes *et al.,* 2002; Batra *et al.,* 2007; Gupta *et al.,* 2008). 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.,* ; Lin and Zhao 2005; Koochi *et al.,* 2011b, 2011c) .

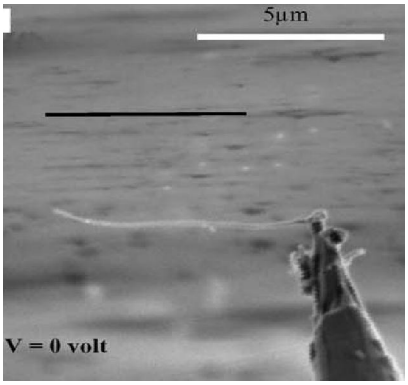

Fig. 1. SEM images of a freestanding CNT probe (Ke *et al.,* 2005a)

In this paper, we utilize a hybrid continuum model to investigate the molecular force-induced deflection and buckling of the cantilever freestanding MWCNT probes/actuators with small number of layers suspended over graphite. The numerical finite difference method is implied to simulate the instability of MWCNT and the obtained results are compared with numerical data.

2. Theoretical Model

2.1. van der Waals interactions

Consider a typical freestanding MWCNT near a surface consisted of N graphene layers, with interlayer distance d = 3.35 Å (figure 2). The length of MWCNT is L, the number of walls of nanotube is N_W, the mean value of their radii is R_W and the gap between MWCNT and the surface is D. A continuum model has been established to compute the van der Waals energy by double-volume integral of Lennard-Jones potential in Refs. (Desquenes *et al.,* 2002; Lennard-Jones, 1930; Girifalco *et al.,* 2000; Ke and Espinosa 2006). In most applications it is practically assumed that the mean radius of MWCNT is much smaller than the distance between nanotube and the graphene surfaces. According to this assumption and using the mentioned continuum model, the intermolecular force per unit length of MWCNT, q_{vdW}, is simplified to (Desquenes *et al.,* 2002):

$$q_{vdW}(r) = 4C_6\sigma^2\pi^2 N_W R_W \sum_{r=D}^{D+(N-1)d} \frac{1}{r^5}. \quad (1)$$

In the above equation, C_6 = 15.2 eVÅ^6 is the attractive constants for the carbon-carbon interaction, (Girifalco *et al.,* 2000) and $\sigma \cong 38\text{nm}^{-2}$ (Desquenes *et al.,* 2002) is the graphene surface density.

In characterizing ultra-thin films/layers by AFM nano-probes, the investigation of MWCNT behavior near a small number of layers can be treated as an important dilemma (Nemes-Incze et al., 2008; Koszewski et al., 2008; Švorčík et al., 2009). Therefore, this study is focused on this case which is very important in engineering problems. In order to derive a simple formula for a small number of layers we substitute r with $D + Nd/2 + id$ and assume $D + Nd/2 \pm id \approx D + Nd/2$. Therefore we get:

$$\sum_{r=D}^{D+(N-1)d} \frac{1}{r^5} = \sum_{i=-N/2}^{N/2} \frac{1}{(D+Nd/2+id)^5} \approx \frac{N}{(D+Nd/2)^5}. \quad (2)$$

This leads to:

$$q_{vdW}(D) \approx 4C_6\sigma^2\pi^2 NN_W R_W (D+Nd/2)^{-5}. \quad (3)$$

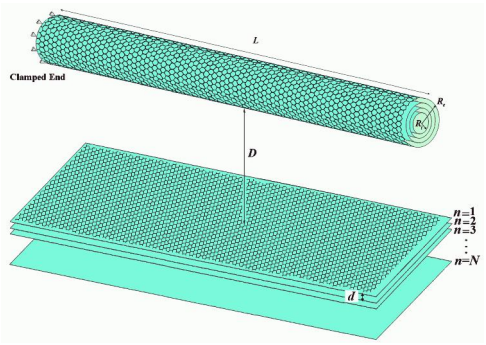

Figure 2. Equivalent continuum model: a MWCNT over a graphite ground plane

2.2. 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 (Gupta *et al.,* 2008) and the cross-sectional moment of inertia I is equal to $\pi(R_o^4-R_i^4)/4$ (Girifalco *et al.,* 2000). We have applied Euler theory to investigate the static elastic behavior of MWCNT. For MWCNTs with $L/(2R_e) > 10$, Euler theory provides fine results compared to those by MM simulations (Batra *et al.,* 2007; Ke *et al.,* 2005b). The effect of large displacement (finite kinematics) is not considered to derive the governing equation of MWCNT. The governing equation of a cantilever MWCNT can be defined as a boundary value problem:

$$E_{eff} I \frac{d^4U}{dX^4} = q_{vdW}(D-U) = \frac{4C_6\sigma^2\pi^2 NN_W R_W}{(D-U+Nd/2)^5} \quad (4a)$$

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

(Geometrical B.C. at fixed end) (4b)

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

(Natural B.C. at free end) (4c)

where X is the position along MWCNT measured from the clamped end and U is the deflection of MWCNT. Equations (4a)-(4c) can be made dimensionless using the following substitutions:

$$x = X/L, \quad (5a)$$

$$u = \frac{U}{D+Nd/2}, \quad (5b)$$

$$f_n = \frac{4C_6\sigma^2\pi^2 NN_W R_W L^4}{E_{eff} I (D+Nd/2)^6}. \quad (5c)$$

These transformations yield,

$$\frac{d^4u}{dx^4} = \frac{f}{(1-u(x))^5}, \quad (6a)$$

$$u(0) = u'(0) = 0, \text{ at } x = 0 \quad (6b)$$

$$u''(1) = u'''(1) = 0, \text{ at } x = 1. \quad (6c)$$

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

3. Numerical Solution

In order to solve the boundary value problem of Eq. 6 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:

$$\frac{d^4u}{dx^4} = \frac{u_{i-2} - 4u_{i-1} + 6u_i - 4u_{i+1} + u_{i+2}}{h^4} \quad (7)$$

where h is the grid spacing, w_i is the deflection of i^{th} grid. By substituting equation 7 in equation 5 we can obtaine:

$$\frac{u_{i-2} - 4u_{i-1} + 6u_i - 4u_{i+1} + u_{i+2}}{h^4} = F_i \quad (8)$$

where

$$F_i = \frac{f}{(1-u_i)^5} \quad (9)$$

Applying equation (8) to all of the elements and incorporating the boundary conditions (eq 6-b and 6-c), a matrix form equation is obtained as:

$$[A]\{u\} = \{F\} \quad (10)$$

Where

$$\{u\} = [u_1, u_2, ..., u_n]^T, \quad (11)$$

And

$$\{F\} = [F_1, F_2, ..., F_n]^T \quad (12)$$

and A matrix can be defined as:

$$[A] = \begin{bmatrix} 7 & -4 & 1 & 0 & 0 & \dots & 0 & 0 & 0 & 0 \\ -4 & 6 & -4 & 1 & 0 & \dots & 0 & 0 & 0 & 0 \\ 1 & -4 & 6 & -4 & 1 & \dots & 0 & 0 & 0 & 0 \\ 0 & 1 & -4 & 6 & -4 & \dots & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & -4 & 6 & \dots & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & -4 & \dots & 0 & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & 0 & \cdots & -4 & 6 & -4 & 1 \\ 0 & 0 & 0 & 0 & 0 & \cdots & 1 & -4 & 5 & -2 \\ 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 1 & -2 & 1 \end{bmatrix} \quad (13)$$

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

5. Results and Discussion

For any given MWCNT-graphite attraction (f), one can solve equation (8a) numerically to obtain the deflection (u) of MWCNT. However, for f greater than critical value of intermolecular force, i.e. f^*, no numerical solution exists and the MWCNT collapses.

Figure 3 shows the centerline deflection of a typical MWCNT under intermolecular force obtained using FDM solution. As seen, u_{tip} increases from zero to u_{tip}^*, when f raises from zero to f^*.

The relations between f and u_{tip} are presented in figure 4. When intermolecular attraction exceeds the critical value f^*, no solution exists for u_{tip} and the instability occurs.

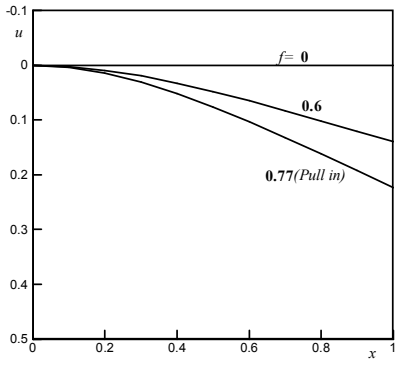

Figure 3. Deflections of the cantilever CNT for different values of intermolecular force (f_n). Collapse occurs when f_n reaches values greater than its critical one, i.e. f^*

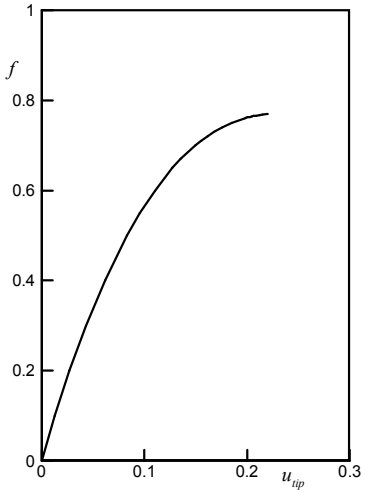

Figure 4. Relationship between f and the MWCNT tip deflection. Collapse occurs when $f$reaches values greater than f^*.

5. Conclusions

In summary, a nano-scale continuum model based on Lennard-Jones potential has been employed to investigate the buckling of cantilever MWCNT with small number of layers over graphene layers. Results indicate that van der Waals attraction can collapse the cantilever MWCNT at submicron separations especially in the case of small number of graphene layers. The proposed approach are capable of predicting the critical values of MWCNT-graphite attraction and MWCNT deflection at the onset of instability. The developed approach avoids time-consuming MM simulations and makes parametric

Corresponding Author:
Alireza Yekrangi
Mechanics group, Ramsar Branch, Islamic Azad University, Ramsar Iran
Email: Yekrangi_ali@yahoo.com

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