The Instability of Multi Walled Carbon Nanotube Probes near Graphite Sheets

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Abstract: In this paper the 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 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. Minimum nanotube-graphite initial gap and stable length of freestanding CNT are determined as basic parameters for engineering applications and nano-devices design. The stable length of MWCNT is determined as a function of its geometrical and material characteristics, initial gap and number of graphene layers.

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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 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 large 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).

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 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

Lennard-Jones potential is a suitable model to describe van der Waals interaction [23]. It defines the potential between atoms *i* and *j* by

$$\phi_{ij} = \frac{C_{12}}{r_{ij}^{12}} - \frac{C_6}{r_{ij}^{6}} \qquad (1)$$

.

where 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 (Desquenes *et al.,* 2002). 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) [25], that is

$$E_{vdW} = \int_{\upsilon_1}\int_{\upsilon_2} n_1 n_2 \left(-\frac{C_6}{r^6(\upsilon_1,\upsilon_2)}\right) d\upsilon_1 d\upsilon_2 \qquad (2)$$

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. (2) provides acceptable results for explaining the CNT-graphene attraction compared to that of direct pair wise summation through molecular dynamics in Eq. (1). 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):

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

The prediction of the stable length and the minimum gap of freestanding MWCNT over a large number of graphene layers are essential in nano-devices (Desquenes *et al.,* 2002; Ke *et al.,* 2005a). Therefore, this study is focused on this case which is very important in engineering problems. For large number of layers, i.e. $D + (N\text{-}1)d >> D$, substitution of the summation with an integral results:

$$\sum_{r=D}^{D+(N-1)d} \frac{1}{r^5} \approx \frac{1}{d}\int_{D}^{D+(N-1)d} \frac{1}{r^5} dr \qquad .(2)$$

$$= \frac{1}{4d}\left[\frac{1}{D^4} - \frac{1}{(D+(N-1)d)^4}\right] \approx \frac{1}{4dD^4}$$

Lastly we have:

$$q_{vdW}(D) \approx C_6\sigma^2\pi^2 N_W R_W d^{-1} D^{-4}. \qquad (3)$$

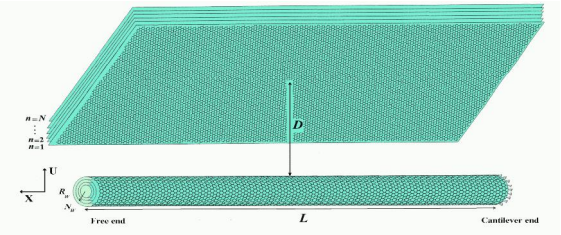

Figure 1. Equivalent continuum model: a MWCNT over a graphite ground plane

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 $\pi(R_o^4\text{-}R_i^4)/4$ (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:

$$E_{eff} I \frac{d^4U}{dX^4} = q_{vdW}(D-U) = \frac{C_6\sigma^2\pi^2 N_W R_W}{d(D-U)^4} \qquad (4a)$$

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

(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:

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

$$u = \frac{U}{D}, \qquad (5b)$$

$$f_n = \frac{C_6\sigma^2\pi^2 N_W R_W L^4}{dE_{eff} ID^5}. \qquad (5c)$$

These transformations yield,

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

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

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

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:

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

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:

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

where

$$F_i = \frac{f}{(1-u_i)^4} \qquad (9)$$

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:

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

Where

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

And

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

and A matrix can be defined as:

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

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

4. Results and Discussion

For any given MWCNT-graphite attraction (f), one can solve equation (6a) 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.

As a case study, a cantilever SWCNT probe/switch with Young's modulus of 1 TPa (Strus *et al.,* 2008) is considered. In this case, I is approximated to $\pi t R_W^3$, where t is the thickness of SWCNT, typically about 0.35 (Strus *et al.,* 2008). Figure 2 depicts the variation of SWCNT stable length as a function of the nanotube radius and minimum initial nanotube-graphite gap. As seen, the intermolecular attraction is more significant for SWCNT over thick graphite substrate compared to that of thin substrate. Figure 2 indicates that the effect of van der Waals attraction on MWCNT's buckling is very important at separations below 1μm.

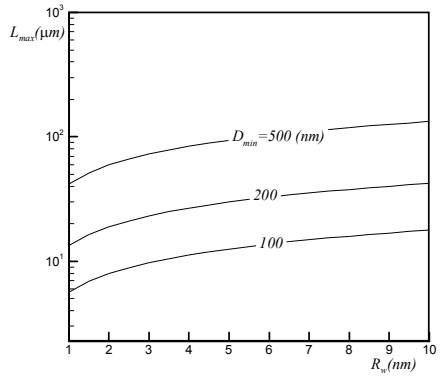

Figure 2. Detachment length of the SWCNT as a function of the nanotube radius for various minimum gaps

5. Conclusions

In summary, a nano-scale continuum model based on Lennard-Jones potential has been employed to investigate the buckling of cantilever MWCNT over graphene layers. Results indicate that van der Waals attraction can collapse the cantilever MWCNT at submicron separations especially in the case of large number of graphene layers. stable length of MWCNT has been determined as basic parameters for design and selecting components of nano-systems. It is found that the stable length of MWCNT highly depends on geometrical dimensions of MWCNT such as radius and number of walls, MWCNT-graphite distance and number of graphene layers. The developed approach avoids time-consuming MM simulations and makes parametric studies possible.

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