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Parameterization of Continuum Theories for Single Wall Carbon Nanotube Switches by Molecular Dynamics Simulations

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Abstract. We propose continuum models for simulation of carbon nanotube based electromechanical switches. Mechanical behavior of a single wall nanotube has been modeled by a continuum model parameterized by using molecular dynamics simulations. By coupling the continuum mechanical and electrostatic models, electromechanical analysis of a single wall nanotube is performed to compute the pull-in voltage.

Keywords: single wall carbon nanotube, NEMS, pull-in voltage, molecular dynamics, continuum theory

1. Introduction

Carbon nanotubes are promising materials for the design and development of nanoelectromechanical Systems (NEMS) and a variety of other nanosystems because of its structural perfection, excellent mechanical and electrical properties, and because of the recent progress made in the fabrication of carbon nanostructures. Since nanosystems typically comprise only a few hundred to thousand atoms, the use of continuum theories might not be accurate to predict the nanodevice behavior. Thus, atomistic simulations such as molecular dynamics simulations are widely used to probe the mechanical and electrical behavior of nanosystems. Many recent studies have, however, demonstrated the possible use of continuum theories for multiwall carbon nanotubes (MWNT) (Ru 2000). The use of single wall carbon nanotubes (SWNT) for NEMS is appealing. However, since a single wall tube comprises only one layer of atoms, continuum theories that are well calibrated for MWNT may not be applicable for SWNT. In this article, we address the development of continuum theories for single wall nanotube based NEMS. Specifically, we show that parameterized continuum models can be used reliably to simulate NEM switches. The contributions of this paper include:

1. The formulation of a continuum model for single wall carbon nanotubes.
2. The extraction of parameters for single wall nanotube mechanics by using molecular dynamics simulations.
3. The application of the parameterized continuum theory for pull-in voltage prediction of NEM switches.

The rest of the paper is organized as follows: In Section 2 we discuss the parameterization of continuum theories. In Section 3 molecular dynamics simulation of carbon nanotubes is presented. In Section 4, the parameterized model is used for electromechanical analysis of a single wall nanotube switch to compute the pull-in voltage. Finally, conclusions are presented in Section 5.

2. Parameterization of Continuum Theories

The validity of continuum theories is questionable at nanoscale and care should be exercised when using them. Continuum theories, such as the beam theory, have been shown to be accurate for mechanical behavior of multiwall nanotubes (tubes with radius of 50 nm) (Treacy, Ebbesen and Gibson 1996) as these tubes could still be considered as bulk material. However, nanotubes with one layer of atoms may not be treated as bulk material as the mechanical properties (such as the Young's modulus, moment of inertia, etc.) characterizing the SWNT could be different from that of a bulk graphite. With a SWNT the primary difficulty arises in defining the cross-section of the tube. In order to study the mechanical behavior of SWNTs we have to define mechanical properties that do not depend on the thickness of the wall. In a recent study (Hernández *et al*. 1998), the Young's modulus of the tube has been retrieved by an approach that is independent of the thickness of the tube. Specifically, in Hernández *et al*. (1998), the strain energy is calculated as a function of the strain, and the Young's modulus is retrieved by computing the second derivative of the energy with respect to the strain. This second derivative is shown to be equal to the Young's modulus times the radius of the tube. Studies on the buckling of nanotubes by a continuum beam model and comparisons with the molecular dynamics simulations highlight the applicability of continuum theories for the prediction of nanotube mechanical behavior (Harik 2001, Yakobson, Brabec and Berholc 1996). Comparing with experiments, the beam equation has been shown to model accurately the deflection of carbon nanotubes (Salvetat *et al.* 1999). The use of a beam model requires the definition of the Young's modulus and the moment of inertia of the SWNT. For a single layer of atoms, the definition of moment of inertia is not trivial as the thickness of the tube is not well defined. Instead of trying to define the Young's modulus and the moment of inertia separately, the approach taken in this paper is to parameterize the product $E \times I$, where E is the Young's modulus and I is the moment of inertia.

3. Molecular Dynamics Simulations

Molecular dynamics simulations have been used extensively for the simulation of nanodevices. Since molecular dynamics simulations are expensive, they are not attractive for design or design optimization. Extracting the material properties from molecular dynamics and studying the device design by using a continuum approach will significantly decrease the modeling time.

3.1. Implementation

In molecular dynamics, the positions of the atoms are computed in a classical way by using the Newton's law of motion. The law of motion for an atom in the system is defined by

$$\frac{d^2 r_i}{dt^2} = \frac{F_i}{M_i} \tag{1}$$

where r_i is the position of atom i, F_i is the force applied on atom i, and M_i is the mass of atom i. For an N-body problem, the forces arise from the interactions between the atoms forming the tube. These interactions are mainly bonded interactions and are modeled with a Brenner potential (Brenner 1990). The Brenner potential, with a parameterization for graphite, has been widely used for the simulation of carbon nanotubes. Since we are primarily concerned with SWNTs in this paper, the non-bonded interactions (namely, the van der Waals interactions) are neglected in this study. The non-bonded interactions become important for MWNTs. Equation (1) is integrated in time by using a velocity Verlet algorithm. The total simulation time is in the range of 100 ps with a timestep of 0.1 fs.

3.2. Material Properties for Single Wall Nanotubes

As discussed in Section 2, the parameters used in continuum theories have to be defined regardless of the thickness of the wall. Assuming that the deflection of a SWNT follows a beam equation, one can retrieve the product EI independent of the thickness of the wall. The value of this product is retrieved for a (16, 0) tube, which has a diameter 1.3 nm and a length of 20 nm. A uniform load is applied to the nanotube and the

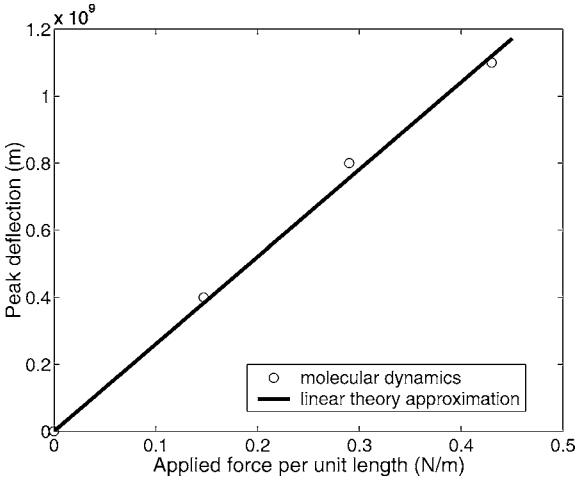

Figure 1. Peak deflection vs. applied force for a (16, 0) fixed-fixed SWNT with a diameter of 1.3 nm and a length of 20 nm. The circles are molecular dynamics data and the solid line is a linear approximation to the data.

nanotube deflection is predicted by molecular dynamics simulation. The peak deflection as a function of the applied load is shown in Fig. 1. A continuum model approximation to the molecular dynamics data requires that the slope of the load-deflection curve be equal to $L^4/(384EI)$, where L is the length of the tube. From the molecular dynamics simulation, the EI product is estimated to be 16×10^{-26} Pa·m^4 for a 1.3 nm diameter SWNT. Shown in Fig. 2 is a comparison of the deflection between molecular dynamics simulations and the parameterized model when a load of 0.43 N/m is applied on the SWNT.

4. Electromechanical Analysis of Carbon Nanotube Based NEMS

Electromechanical analysis of carbon nanotube based fixed-fixed switches has been performed. The van der Waals forces have not been taken into account because it has little influence for a fixed-fixed geometry

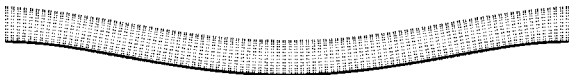

Figure 2. Comparison of the deflection obtained with molecular dynamics and parameterized beam model. A (16, 0) fixed-fixed SWNT with a diameter of 1.3 nm and a length of 20 nm is considered. The solid black line is the deflection predicted by the parameterized beam equation.

(Dequesnes, Rotkin and Aluru 2001). Using the material parameters determined in Section 3, the deflection of a single wall nanotube due to electrostatic forces has been computed using the beam equation.

4.1. Continuum Model

The electromechanical behavior of the SWNT is approximated by a continuum beam equation i.e.

$$EI\frac{d^4y}{dx^4} = q_{elec} \tag{2}$$

where y is the gap between the ground plane and the bottom of the tube at the position x of the beam and q_{elec} represents the electrostatic forces (per unit length). The electrostatic forces are computed by using a standard capacitance model. The nanotube is approximated as a perfect cylindrical conductor. This implies that the potential is constant along the length of the tube. Then, the capacitance per unit length for the cylindrical beam over the conductive ground plane is given by

$$C(r) = \frac{2\pi\epsilon_0}{\log\left[1 + \frac{y}{R} + \sqrt{\left(\frac{y}{R}+1\right)^2 - 1}\right]} \tag{3}$$

where ϵ_0 is the permittivity of vacuum, and R is the radius of the tube. From the electrostatic energy, $E_{elec} = \frac{1}{2}CV^2$, the electrostatic force per unit length, q_{elec}, can be computed by differentiating the energy with respect to the gap y, i.e.

$$q_{elec} = -\frac{\pi\epsilon_0 V^2}{R\sqrt{\frac{y(y+2R)}{R^2}}\log^2\left[1 + \frac{y}{R} + \sqrt{\frac{y(y+2R)}{R^2}}\right]} \tag{4}$$

Equation (2) is a non-linear equation, which implies that there is, in general, no analytical solution. The solution has been obtained numerically by solving Eq. (2) self-consistently. The pull-in phenomenon is also predicted by solving Eq. (2). The electrostatic forces are modulated by the applied voltage, which deflects the cantilever. The deflection of the tube increases with the applied voltage. At a certain voltage, defined as the pull-in voltage, the tube becomes unstable and collapses onto the ground plane as the restoring force does not balance the electrostatic force anymore. Using the EI product obtained from molecular dynamics simulations, the pull-in voltage has been obtained for a SWNT fixed-fixed switch. The SWNT is a (16, 0) tube, which

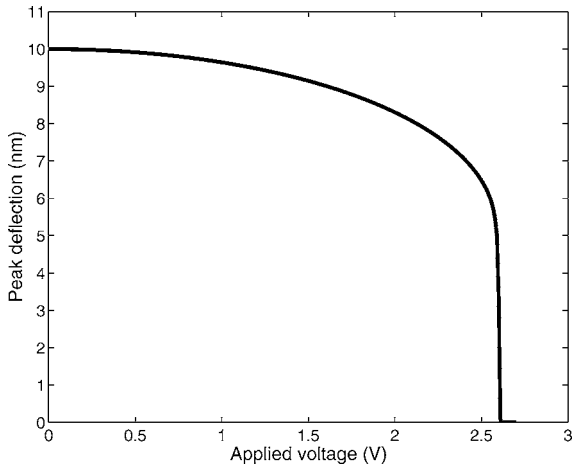

Figure 3. Peak deflection (which is at the center of the nanotube) as a function of the applied voltage for a SWNT fixed-fixed switch.

has a length of 100 nm, diameter of 1.3 nm and is suspended 10 nm above the ground plane. The peak deflection of the SWNT fixed-fixed tube as a function of the applied voltage is shown in Fig. 3. The pull-in voltage is computed to be 2.60 V.

4.2. Lumped Model

The pull-in voltage can be estimated by using a 1D lumped model. In this 1D lumped model the switch is approximated as a rigid beam suspended over a ground plane. The electrostatic force is given by, $F_{elec} = q_{elec} L$, where q_{elec} is given in Eq. (4). The elastostatic force, F_{elas}, is modeled by a spring. Considering a uniformly loaded fixed-fixed beam, the spring constant is defined by the ratio of the applied force to peak deflection. For a deflection of x, the elastostatic force is then given by, $F_{elas} = k(g - x)$, where g is the initial gap. For a fixed-fixed beam, $k = 384\, EI/L^3$. The pull-in voltage can be computed by solving $F_{elec} + F_{elas} = 0$. Assuming that the pull-in occurs at 2/3 of the initial gap, the pull-in voltage with a 1D lumped model is given by

$$V_{PI} = \sqrt{k(g - y_{eq})\left(\frac{R\sqrt{\frac{y_{eq}(y_{eq}+2R)}{R^2}}\log^2\left(1 + \frac{y_{eq}}{R} + \sqrt{\frac{y_{eq}(y_{eq}+2R)}{R^2}}\right)}{\pi\epsilon_0 L}\right)} \tag{5}$$

where $y_{eq} = \frac{2}{3}g$. The pull-in voltage obtained from Eq. (5) for the (16, 0) SWNT fixed-fixed switch considered in the previous section is 2.31 V. The pull-in voltage with the lumped model is underestimated as the forces are overestimated in the lumped model.

5. Conclusion

A continuum model for the simulation of single wall carbon nanotube based nanoelectromechanical switches is proposed in this paper. For the continuum model, the product of Young's modulus and moment of inertia is extracted from molecular dynamics simulations. Using the parameterized beam model, continuum electromechanical simulations have been performed for a fixed-fixed SWNT switch to compute the pull-in voltage. A 1D lumped model is presented to estimate the pull-in voltage of SWNT based NEM switches.

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References

Brenner D.W. 1990. Empirical potential for hydrocarbons for use in simulating the chemical vapor deposition of diamond films. Phys. Rev. B 42(15): 9458–9471.

Dequesnes M., Rotkin S.V., and Aluru N.R. 2002. Calculation of pull-in voltages for carbon nanotube-based nanoelectromechanical switches. Nanotechnology 13: 120–131.

Harik V.M. 2001. Ranges of applicability for the continuum beam model in the mechanics of carbon nanotubes and nanorods. Solid State Comm. 120: 331–335.

Hernández E., Goze C., Bernier P., and Rubio A. 1998. Elastic properties of C and $B_xC_yN_z$ composite nanotubes. Phys. Rev. Lett. 80(20): 4502–4505.

Ru C.Q. 2000. Effective bending stiffness of carbon nanotubes. Phys. Rev. B 62(15): 9973–9976.

Salvetat J.P. *et al*. 1999. Elastic modulus of ordered and disordered multiwalled carbon nanotubes. Advanced Materials 11(2): 161–165.

Treacy M.M.J., Ebbesen T.W., and Gibson J.M. 1996. Exceptionally high young's modulus observed for individual carbon nanotubes. Nature 381: 678–680.

Yakobson B.I., Brabec C.J., and Berholc J. 1996. Nanomechanics of carbon tubes: Instabilities beyond linear response. Phys. Rev. Lett. 76(14): 2511–2514.