Simulation of carbon nanotube-based nanoelectromechanical switches

Marc Dequesnes, S.V. Rotkin and N.R. Aluru
Beckman Institute for Advanced Science and Technology
University of Illinois at Urbana-Champaign
Urbana, IL 61801 USA

ABSTRACT

We study the pull-in voltage characteristics of several multiwall nanotube electromechanical switches such as suspended carbon nanotubes over a graphitic ground lectrode. Electromechanical analysis has been performed by accounting for three coupled energy domains: elastostatics, electrostatics, and van der Waals interactions. We have shown that, by comparing to molecular dynamics simulations, the use of continuum theories for mechanics and van der Waals interactions is justified.

The continuum approach proposed in this work has been used to simulate the behaviour of carbon-nanotube based nano-switches. Several cantilever and fixed-fixed carbon nanotubes over a graphite ground plane have been simulated. The pull-in voltage calculations for a cantilever switch and a fixed-fixed switch emphasize the significance of van der Waals forces in nanoelectromechanical switches.

Keywords: carbon nanotube, NEMS, pull-in voltage

1 INTRODUCTION

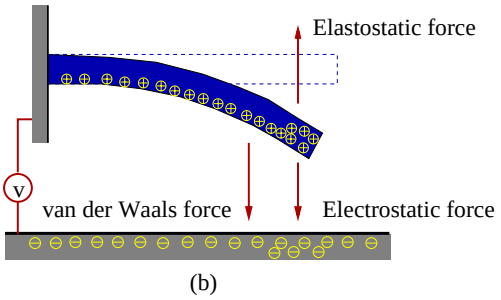
Nanoelectromechanical Systems (NEMS) are nanoscale sensors, actuators, devices and ystems. NEMS are about a 1000 times smaller than Microelectromechanical Systems (MEMS). NEMS has the potential to enable revolutionary technology for sensing, actuation, computing and information technology. Some NEMS applications that have already been demonstrated include the development of random access memory [1] and nanotweezers [2]. Both these devices use a carbon nanotube based nanoswitch as a fundamental building block. In this paper, we report on electromechanical behavior of nanoscale switches. The mechanical and electromechanical behavior of nanotubes can be investigated by using molecular dynamics simulations. For example, the mechanics of nanogears have been investigated using molecular dynamics simulations [3]. However, atomic scale simulations, such as molecular dynamics, are very expensive and may not be easily integrated into a design process. In this paper, by performing rigorous validation with molecular dynamics simulations, we propose the use of continuum theories for nanoelectromechanical (NEM) switches.

The operation and design of NEM switches closely resembles the design and operation of microelectromechanical (MEM) switches. Hence, the obvious question is can MEMS theories be used to design NEMS? Because NEM switches are about three orders of magnitude smaller than MEM switches, new physics is encountered when designing NEM switches. Specifically, van der Waals interactions, which can be neglected when designing MEM switches, play an important role at nanoscales. Hence, the use of MEMS models is limited and new models need to be developed for analysis and design of NEM switches.

In this article we raise the question of applicability of continuum theories for nanoscale devices. NEM switches are typically designed with small gaps between the tubes and the ground plane. In such cases, we show that parameterized continuum models can be used reliably to design nanoscale devices.

2 OPERATION OF NEM SWITCHES

Shown in Figure 1 is the physical operation of a carbon nanotube based cantilever switch. The key components are a movable structure, which can be a single wall or a multiwall carbon nanotube, and a fixed ground plane, which is modeled by a graphite bulk. When a potential difference is created between the movable structure and the ground plane, electrostatic charges are induced on both the movable structure and the ground plane. The electrostatic charges give rise to electrostatic forces which deflect the movable tube. In addition to electrostatic forces, depending on the gap between the movable tube and the ground plane, van der Waals forces also act on the tube and deflect it. The direction of the electrostatic and van der Waals forces is shown in Figure 1. Counteracting the electrostatic and van der Waals forces are elastic forces, which try to restore the tube to its original straight position. For an applied voltage, an equilibrium position of the tube is defined by the balance of the elastic, electrostatic and the van der Waals forces. When the applied potential difference between the tube and the ground plane exceeds a certain potential, the tube becomes unstable and collapses onto the ground plane. The potential which causes the tube to collapse onto the ground plane is defined as the



(b)

Figure 1: Force balance for a nanotube over a ground plane when $V \neq 0$ (the dotted line represents the undeformed position of the tube when $V = 0$).

pull-in voltage or the collapse voltage.

When compared to microelectromechanical switches, the operation of nanoelectromechanical switches is different because of the importance of the van der Waals forces, which can be neglected at the micrometer scale. In this paper, we show that the van der Waals forces can have a significant effect on the calculated pull-in voltage of NEM switches.

3 THEORY

3.1 Van der Waals interactions

The van der Waals energy can be computed by using the well-known Lennard-Jones potential. In the continuum model, the total van der Waals energy is computed by the double volume (or surface) integral of the Lennard-Jones potential. To compute the interaction of a multiwall nanotube (MWNT) with a bulk graphite (see Figure 2) we sum the terms defining the interaction between all separate shells and layers. For a MWNT, the energy per unit length is given by

$$q_{vdW} = \sum_{R=R_{int}}^{R_{ext}} \sum_{r=r_{init}}^{(n-1)\times d + r_{init}} -\frac{\mathcal{C}_6 \sigma^2 \pi^2 R \sqrt{r(r+2R)}}{2r^5(r+2R)^5} \times \left(8r^4 + 32r^3R + 72r^2R^2 + 80rR^3 + 35R^4\right) \quad (1)$$

where $\sigma \simeq 38\,\mathrm{nm}^{-2}$ is the graphite surface density, $\mathcal{C}_6 = 15.2\,eV.\mathring{A}^6$ is the Lennard-Jones attractive constant, R_{int} and R_{ext} are the inner and the outer radius of the nanotube, respectively, n is the number of graphene layers of the substrate, $d = 3.35\mathring{A}$ is the interlayer distance of graphite and r_{init} is the gap between the outer wall of the nanotube and the surface layer of graphite. More details on how Equation (1) has been derived is given in [4].

3.2 Electrostatic forces

The electrostatic forces are computed by using a standard capacitance model. The nanotube is approximated as a perfect cylindrical conductor. The electrostatic force per unit length for the cylindrical beam over the conductive ground plane, q_{elec}, is then given by

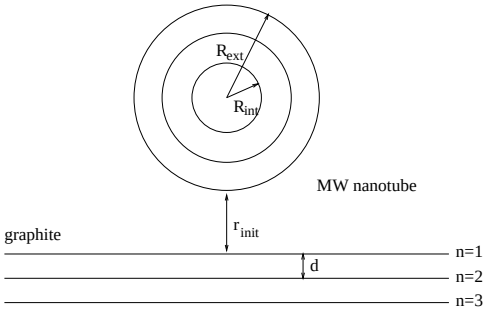


Figure 2: Multiple shell continuum geometry: a MWNT over a graphite ground plane.

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

where R is the radius of the cylinder/conductor ($R = R_{ext}$ for MWNT), r is the gap between the conductor and the ground plane ($r = r_{init}$ for the configuration shown in Figure 2), and ϵ_0 is the permittivity of vacuum.

3.3 Governing equation for NEM switches

The pull-in voltage of the nano cantilever and the fixed-fixed tube device can be determined by coupling the electrostatic, van der Waals and elastostatic domains into a single equation, i.e.

$$EI\frac{d^4r}{dx^4} = q_{elec} + q_{vdW} \quad (3)$$

where r is the gap between the conductor and the ground plane, x is the position along the tube, E is the Young's modulus and I is the moment of inertia. For nanotubes with an interior radius R_{int} and an exterior radius R_{ext}, I can be estimated as:

$$I = \pi/4 \times (R_{ext}^4 - R_{int}^4) \quad (4)$$

The expressions for q_{vdW} and q_{elec} are given in Equation (1) and Equation (2), respectively. The governing equation is non-linear, which means that it is not possible, in general, to come up with an analytical solution. It is to be solved self-consistently to compute the equilibrium position of the nanotubes. Starting with an initial guess for the deflection of the tube, the forces are computed and, then, are used to solve the equation to compute a new deflection of the tube. These steps are repeated till a converged solution is obtained.

4 VALIDITY OF THE CONTINUUM BEAM THEORY

In order to test the accuracy of beam theories for multiwall nanotubes, molecular dynamics simulations have been performed on a double wall nanotube (DWNT) with a diameter of 1.96 nm and a length of 20 nm at 10 K. The DWNT considered is made of a (25,0) tube for the outer shell and a (16,0) tube for the inner shell. The bonded and non-bonded interactions are modeled respectively by a Brenner potential [5] and by a Lennard-Jones potential. For a uniformly distributed load of 1.8 N/m, the comparison between the beam theory given in Equation (3) (with a constant right hand side or forcing term) and the molecular dynamics simulations is shown in Figure 3. The agreement is excellent for an I computed by using Equation (4), where $R_{int} = 6.3\,\mathring{A}$ and $R_{ext} = 9.8\,\mathring{A}$. The Young's modulus was set to be 1.2 TPa as determined from the molecular dynamics simulations.

To determine the Young's modulus, the peak deflection of the tube as a function of the applied load is plotted as shown in Figure 4. A continuum model approximation for the load-deflection curve shown in Figure 4, requires that the slope be equal to $L^4/(384EI)$, where L is the length of the tube. From the slope of the MD load-deflection curve, the Young's modulus of the tube is retrieved to be $E \simeq 1.2$ TPa. This value is consistent with the theoretical and experimental data published previously.

From Figure 4, it can be noticed that the deflection for larger loads can no longer be modeled by a linear theory. Another deviation from the beam theory is observed for very large loads. This deviation is the buckling of nanotubes which arises because of stress concentration at the edges. These are the main limitations of our mechanical model.

5 RESULTS AND DISCUSSION

5.1 Nanotweezers problem

The first example we investigate is the nanotweezers problem. Experimental data on the nanotweezers problem has been reported recently in [2]. The length of the tweezers is 2.5 μm and the gap between the two tweezers is 780 nm. The diameter of the nanotube was not experimentally measured. Akita *et. al.* [2] theoretically estimated a diameter of 13.3 nm. The Young's modulus has been taken to be 1 TPa in [2].

The inset in Figure 5 shows the geometry used in our calculations. Using the continuum model presented in this paper, we were able to obtain a good match with experimental data with a diameter of 10.9 nm. Because of the large gap between the two tweezers, the van der Waals forces are negligible. The tip deflection as a function of the applied voltage is shown in Figure 5. The experimental data from [2] is also shown in Figure 5. The computed pull-in voltage is 4.65 V. The above example demonstrates that our continuum model does a reasonably good job in predicting the electromechanical behavior of nanotweezers.

Figure 3: Comparison of the deflection of a 20 nm long fixed-fixed double wall nanotube with the deflection predicted by the beam equation. The solid black line is the deflection predicted by the beam equation.

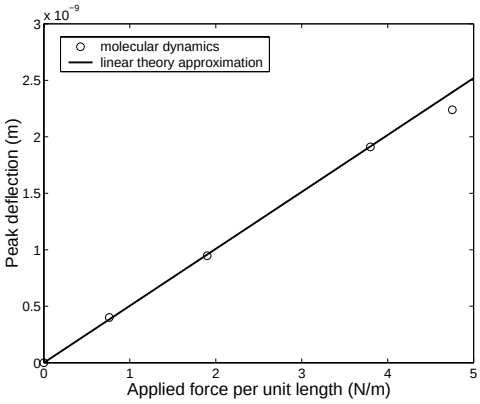


Figure 4: Peak deflection vs. applied force for a fixed-fixed DWNT with a diameter of 1.96 nm and a length of 20 nm. The circles are molecular dynamics data and the solid line is a linear approximation to the data.

5.2 Cantilever switch

The next example we consider is a DWNT cantilever switch. The geometry of the switch is shown as inset in Figure 6. The DWNT is 50 nm long, and has a diameter of 2 nm ($R_{ext} = 10\,\mathring{A}$ and $R_{int} = 6.65\,\mathring{A}$) and is positioned 4 nm above the ground plane. The tip deflection as a function of the applied voltage is shown in Figure 6. When the van der Waals forces are neglected, the pull-in voltage is 0.97 V. When the van der Waals forces are taken into account, the pull-in voltage reduces to 0.48 V.

We have repeated the same simulation with a larger gap (10 nm) but with the same length and diameter. The pull-in voltage is computed to be 3.0 V and 3.1 V, respectively, with and without the van der Waals forces. In this case, we have noticed that the effect of the van der Waals interaction is negligible. From this example, we can conclude that for smaller gaps the van der Waals forces play an important role in determining the deflections as well as the pull-in voltage of cantilever switches.

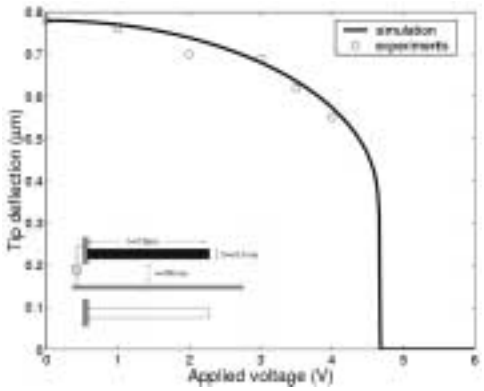


Figure 5: Tip deflection as a function of the applied voltage for a nanotweezers problem. Inset: The model geometry.

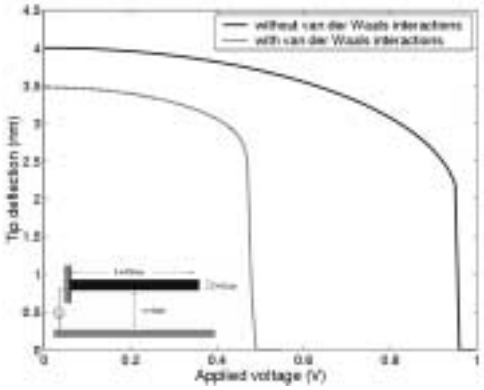


Figure 6: Tip deflection as a function of the applied voltage for a cantilever switch. Inset: The geometry of the cantilever switch.

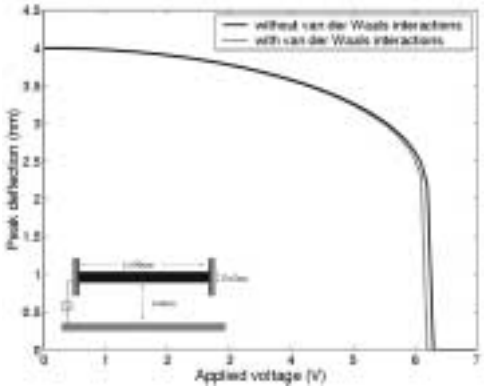


Figure 7: Peak deflection (which is at the center of the nanotube) as a function of the applied voltage for a fixed-fixed switch. Inset: The geometry of the fixed-fixed switch.

5.3 Fixed-fixed switch

We have also simulated a DWNT fixed-fixed switch with a length of 50 nm, diameter of 2 nm and a gap of 4 nm. The geometry is shown as inset in Figure 7. Compared to a cantilever geometry, fixing both ends of the tube makes the tube stiffer and results in smaller deflections. The results for the fixed-fixed switch are summarized in Figure 7. First, we observe that the pull-in voltage required to collapse the fixed-fixed tube is 6.3 V, which is much higher compared to the cantilever switch. In addition, we observe that the van der Waals interactions are not significant. The pull-in voltage computed by including the van der Waals forces is 6.2 V. From this example, we can conclude that even at a small gap, the van der Waals interactions are not significant for fixed-fixed tubes.

6 CONCLUSION

A continuum model for the simulation of carbon nanotube based nanoelectromechanical switches is proposed in this paper. In particular, a parameterized beam model is shown to provide good results for mechanical behavior of NEM switches. The Young's modulus required in the beam equation is extracted from molecular dynamics simulations. Numerical results with the continuum model for a nanotweezers problem compare well with the experimental data. Pull-in voltages for cantilever and fixed-fixed double wall nanotube switches are computed by using the continuum model. Results indicate that the van der Waals force can play a significant role in determining the pull-in voltage of cantilever switches for small gaps. A fixed-fixed switch is less sensitive to the van der Waals force and can operate with much smaller gaps.

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