Deformation characterization of a nanoelectromechanical switch

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Abstract. This paper analyses the deformation of a double-walled nanotube-based nanoelectromechanical switch. The product of Young’s modulus and moment of inertia of the tube is determined by a molecular dynamics simulation with a linear deflection approximation. The switch is simplified to a beam system, and the loading is calculated from three coupled energy domains: the electrostatic energy domain, the elastostatic energy domain, and the van der Waals energy domain. A meshless formulation is then used to discretize the switch to establish the non-linear system of equations for analysis. A parametric comparison with the results in the literature showed that the method developed in this paper is very effective.

1. Introduction

The increasing interest in nanotechnology has influenced the development of microelectromechanical systems (MEMS). A new class of MEMS devices being developed at the nanoscale is called nanoelectromechanical systems (NEMS). The NEMS device is about a thousand times smaller than MEMS, and has a promising potential in practical applications in, e.g., random access memories, nanotweezers for miniaturized robots, and nanoswitches, where carbon nanotubes are often used because of their excellent electronic and mechanical properties.

Owing to their small dimensional scale, experiments on nanoswitches are costly. Numerical simulations have therefore become an important tool for their analysis and design. The molecular dynamics (MD) method, though often used presently, requires a significant computational cost, and hence necessitates the investigation of some alternative ways, such as the semi-analytical and analytical methods[1,2]. However, the limitations of these methods when applying to NEMS are obvious, especially in the case of complex devices.

This paper will develop a new method for the characterization of NEMS, demonstrated by analyzing the deformation of a nanoelectromechanical (NEM) switch, as shown in figure 1, whose key components are a double-walled carbon nanotube (DWNT) and a fixed ground plane. When a potential difference is created between the nanotube and the ground plane, electrostatic charges, which will lead to electrostatic force, are introduced. Meanwhile, elastostatic and van der Waals forces co-exist. Under an applied voltage, an equilibrium position of the tube is defined by the balance of the elastostatic, electrostatic and the van der Waals forces. To simulate this NEM switch, we can use a parameterized continuum model, with the product of the DWNT’s Young’s modulus and moment of
inertia determined by an MD simulation and a linear deflection approximation. To do so, the switch is simplified to a beam system, and the loading is calculated from three coupled energy domains: the electrostatic energy domain, the elastostatic energy domain, and the van der Waals energy domain. A meshless formulation\cite{3,4} is then developed to discretize the domain of the switch to establish the non-linear equations for deformation analysis.

**Figure 1.** A DWNT-based NEM switch. (a) voltage $V = 0$; (b) voltage $V > 0$

2. **Modelling**

1) The elastostatic domain
The nanotube in the switch can be simplified to a beam structure. According to the continuum theory, the governing equation for the beam can be written as

$$E I \frac{d^4 w}{dx^4} = f$$

where $w$ is the deflection of the nanotube, $E$ is its Young’s modulus, $I$ is its moment of inertia, and $f$ is the force per unit length on the tube.

For a cantilever tube, as shown in figure 1, there are four boundary conditions, two at each end. The boundary conditions are given at the global boundary, $\Gamma$, as

$$w(0) = 0, \quad \theta(0) = 0, \quad M(l) = 0, \quad Q(l) = 0,$$

at the fixed end

$$\theta(l) = 0, \quad Q(l) = 0,$$

at the free end

where $\theta$, $M$ and $Q$ denote the deflection slope, the bending moment and the shear force, respectively, and $l$ is the length of the tube.

2) The electrostatic force
The electrostatic force can be computed by using a standard capacitance model\cite{5}, in which the nanotube is considered as a perfect cylindrical conductor. This implies that the potential is constant along the length of the tube. The electrostatic force per unit length can be written as

$$f_e = -\varepsilon_0 V^2 \left\{ g \left\{ g(2r_i) / r_i^2 \right\}^{-1/2} \log \left\{ 1 + g / r_i + \left[ g(2r_i) / r_i^2 \right]^{-1/2} \right\} \right\}$$

where $\varepsilon_0$ is the permittivity at vacuum, $g$ is the gap between the nanotube and ground plane, and $V$ is the voltage applied.

3) The van der Waals interaction
The van der Waals force can be computed through the van der Waals energy using an atomistic potential. The Lennard-Jones (L-J) potential is used in this paper. In the L-J potential, there are attractive and repulsive parts. The repulsive part decays very fast and plays an important role only when the nanotube is to contact with the ground. Hence, it is reasonable to consider the attractive part...
in the calculation of the van der Waals energy $W$ using a pair-wise summation over all the atoms. As shown in figure 2, a DWNT interacts with $m$ layers of graphene in the substrate, and if the interlayer distance of the graphene is $d$, the van der Waals force of the DWNT can be written as

$$f_z = -\sum_{i=1}^{m} \left[ C \sigma^2 \pi^4 r_i^2 \left( g_i (g_i + 2r) \right) \left( 8g^4 + 32g^3 r_1^2 + 72g^2 r_1^2 r_2^2 + 80g^2 r_1^2 r_2^2 + 35r_1^2 r_2^2 \right) \right]^{-1} +$$

$$\left[ C \sigma^2 \pi^4 r_i^2 \left( g_i (g_i + 2r) \right) \left( 8g^4 + 32g^3 r_1^2 + 72g^2 r_1^2 r_2^2 + 80g^2 r_1^2 r_2^2 + 35r_1^2 r_2^2 \right) \right]^{-1}$$

where $C$ is a constant characterizing the interactions between two atoms, $\sigma$ is the graphite surface density, $g = g + d \times (i - 1)$, and $r_0$ and $r_1$ are the radii of the inner and outer nanotubes of the DWNT.

The total force in equation (1), $f$, is therefore $f = f_i + f_z$.

**Figure 2.** A DWNT over a graphite ground plane

**Figure 3.** The weight domain $\Omega_w$ and quadrature domain $\Omega_q$ for node $I$; support domain $\Omega_s$ for Gauss integration point $x_Q$

4) Young’s modulus and moment of inertia

To use the above continuum model, Young’s modulus, $E$, and moment of inertia, $I$, of the DWNT should be determined. There have been some confusions in determining the Young’s modulus of a nanotube due to the dilemma of the effective thickness, $h$. Vodenitcharova and Zhang$^6$ pointed out the equivalent thickness of a single-walled carbon nanotube should be 0.617 Å, which is 43.8% of the theoretical diameter of a carbon atom, and its Young’s modulus is 4.88 TPa. However, there is not a rational value of wall-thickness for a DWNT available that can be used to determine its $E$ and $I$.

Since this study considers only the linear elasticity of the DWNT with small deflection, its $E$ and $I$ are therefore constants. Hence, the linear deflection approximation, in which the peak deflection of the tube is considered as a linear function of the applied load, can be used to get the product of $E$ and $I$.

The peak deflections for different loadings are first obtained by the MD simulation, and then using the classic beam theory to calculate $EI$. That is, for a cantilever tube, if the peak deflection is $w_d$ (obtained by MD simulation$^{1,8}$) when the force is $f$, we can simply obtain $EI$ as

$$EI = \frac{l^4 f}{8w_d}$$

where $l$ is the length of the tube. To ensure the accuracy, various loading conditions can be used to get several $EI$, and the average value of these $EI$ is considered as the equivalent $EI$. 

3. Local meshless formulation

A local weak form of the differential equation (1), over a local domain \( \Omega \), bounded by \( \Gamma \), can be obtained using the weighted residual method\[3,4]\:

\[
\int_{\Omega} v(Elw^r - f)dx = 0
\]

where \( v \) is the weight function. The first term on the left hand side of equation (8) can be integrated by parts to become

\[
\int_{\Omega} (Elv^r w^r - vf)dx - [\bar{E}Elv'w^r]_\Gamma + [\bar{E}Elvw^r]_\Gamma = 0
\]

where \( \bar{E} \) is the unit outward normal to domain \( \Omega \).

Gauss quadrature is needed to evaluate the integrations in equation (8). As shown in figure 3, for a field node \( x_I \), a local quadrature cell \( q \) is needed for the Gauss quadrature; for each Gauss quadrature point \( x_Q \), the meshless shape functions are constructed to obtain the integrand. Therefore, for a field node \( x_I \), there exist three local domains:

- the local quadrature domain \( \Omega_q \) (size \( r_q \));
- the local weight (test) function domain \( \Omega_v \), where \( v_i \neq 0 \) (size \( r_v \));
- the local support domain \( \Omega_s \) for \( x_Q \) (size \( r_s \)).

These three local domains are arbitrary as long as the condition \( r_q \leq r_v \leq r_s \) is satisfied. It has been noted that when an appropriate weight function is used, the local weak form, equation (9), can be simplified because the terms along the internal boundary vanish. Hence, for simplicity, we can use \( r_q = r_v \).

The problem domain \( \Omega \) is represented by properly scattered field nodes, and the point interpolation\[3\] is used to approximate the value of a point \( x \)

\[
w(x) = \Phi^T_w (x) w + \Phi^T_s (x) \theta
\]

where \( w \) and \( \theta \) denote the nodal deflections and slopes, respectively, and \( \Phi_w(x) \) and \( \Phi_s(x) \) are shape functions for deflection and slope, respectively.

Substituting equation (9) into the local weak form equation (8) for all nodes leads to the following discrete equations

\[
K w^r = f
\]

It can be found from equations (4) and (5) that \( f \) is nonlinear, because it is the function of the deflection. The nonlinear force \( f \) leads to the nonlinearity of equation (10), and thus an iteration technique, the Newton-Raphson method, is required for its solution.

4. Results

A cantilever switch is considered to consist of a DWNT of 50 nm in length, with \( r_1 = 1 \) nm, \( r_0 = 0.665 \) nm. The initial gap between the DWNT and the ground plane is 4 nm. There are 30 sheets of grapheme for the ground plane, and the inter-layer distance of graphite, \( d \), is 0.335 nm. The equivalent \( EI \) is \( 7.58 \times 10^{-21} \) m N, and \( \varepsilon = 8.854 \times 10^{-12} \) C²/Nm²\[5\].

To analyze this switch by the above meshless formulation, 41 regularly distributed field nodes are used. With the increase of the applied voltage, the deflection of the DWNT increases, and the gap between the tube and the ground plane decreases. When the voltage increases to a certain value, the tube becomes unstable suddenly and the free end of the tube will touch the bottom plane. This process is defined as the pull-in behavior and the corresponding voltage value is called the quasi-static critical pull-in voltage, at which the deflection of the tube tip equals to the initial gap. Figure 4 demonstrates the result of the deflection of the tube tip under different voltages. It can be seen that the critical pull-in voltage is 0.474 volt. Compared with the same value, 0.5 volt, obtained by the analytical method\[1\], the presented method gives a very good result. It should be mentioned here that the above model is only valid when the tube deflection is small. However, it can be seen from figure 4 that the model is accurate up to the critical pull-in voltage. The sharp increase of the tube deflection beyond the critical pull-in voltage, as shown in figure 4, is caused by the sharp increase of the forces, as demonstrated in
Because of the decrease of the gap between the DWNT and the ground plane, both the electrostatic and van der Waals forces increase significantly, which pull the tube down suddenly.

The relationship between the critical pull-in voltage and the initial gap for this switch is shown in figure 6. The critical pull-in voltage increases with the increase of the initial gap. When the initial gap is larger than 6 nm, the slope for the curve changes very slowly, because with a large gap, the effect of the van der Waals force is negligible. When the gap is very small, on the other hand, the van der Waals force will play a key role. At a critical gap value ($g \approx 3.5$ nm in the present case), pull-in will occur even without an external voltage.

![Figure 4. The gap under different voltages](image)

![Figure 5. Forces vs. gaps](image)
5. Conclusion
This paper analyses the deformation of a NEM switch using the meshless technique based on a parameterized continuum model. It was found that the method used in this paper is very effective. Meanwhile, the model predicted that the coupling effect of elastostatic and van der Waals forces is important when the gap between the DWNT and the ground is not too small but not too big (between 3.5 nm to 6 nm in the present switch configuration).

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References
[1] Dequesnes M, Rotkin SV and Aluru NR 2003 Calculation of pull-in voltages for carbon-nanotube-based nanoelectromechanical switches Nanotechnology 13 120–131.
[2] Osterberg PM 1995 Electrostatically actuated micromechanical test structures for material property measurement PhD Dissertation MIT (Cambridge, MA).
[3] Liu GR and Gu YT 2005 An Introduction to Meshfree Methods and Their Programming (Springer, Berlin).
[4] Gu YT and Liu GR 2001 A local point interpolation method for static and dynamic analysis of thin beams Computer Method in Applied Mechanics Engineering 190 5515-5528.
[5] Jackson JD 1998 Classical Electrodynamics (3rd edn, Wiley, NewYork).
[6] Wong EW, Sheehan PE and Lieber CMV 1997. Nanobeam mechanics: elasticity, strength, and toughness of nanorods and nanotubes Science 277 1971-1975.
[7] Vodenitcharova T and Zhang LC 2003 Effective wall thickness of a single-walled carbon nanotube Physical Review B 68 165401.
[8] Mylvaganam K and Zhang LC 2004 Important issues in a molecular dynamics simulation for characterizing the mechanical properties of carbon nanotubes Carbon 42, 2025-2032.