

Numerical Analysis of Nanotube Based NEMS Devices

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ABSTRACT

A non-linear analysis of nanotube based nano-electromechanical systems (NEMS) is presented. Singly and doubly clamped nanotubes under electrostatic actuation are examined by solving nonlinear elastic equations. The analysis emphasizes the importance of nonlinear effects, such as finite kinematics (i.e. large deformations) and charge concentrations at the tip of singly clamped nanotubes, in the prediction of the *pull-in* voltage of the device, a key design parameter. We show that nonlinear kinematics results in an important increase in the *pull-in* voltage of doubly clamped nanotube devices, but that it is negligible in the case of singly clamped devices. Likewise, we demonstrate that charge concentration at the tip of singly clamped devices results in a significant reduction in *pull-in* voltage. By comparing numerical results to analytical predictions, closed form formulas derived elsewhere are verified. The results reported in this work are particularly useful in the characterization of the electro-mechanical properties of nanotubes as well as in the optimal design of nanotube based NEMS devices.

1. Introduction

Carbon nanotubes (CNTs) have long been considered ideal building blocks for Nanoelectromechanical systems (NEMS) devices due to their superior electro-mechanical properties. The CNT-based NEMS reported in the literature, such as nanotweezers,¹⁻² nonvolatile random access memory (RAM) devices,³ and feedback-controlled nanocantilever NEMS devices,⁴ can be simply modeled as CNT cantilevers or fixed-fixed CNTs hanging over an infinite conductive substrate. In order to design a functional NEMS device, its electro-mechanical characteristic should be well quantified in advance. Generally, multi-walled carbon nanotubes (MWNTs) can be modeled as homogeneous cylindrical beams and perfect conductors. In this paper, we investigate the electro-mechanical characteristics of singly and doubly clamped CNT-based NEMS, as illustrated in Fig.1: a biased MWNT cylinder of length L , placed above an infinite ground plane, at a height H . The inner radius and outer radius of MWNT are R_{int} and R_{ext} , respectively. The applied voltage between nanotube and substrate is V . In particular, two important but typically omitted effects in the modeling of nano-devices, such as concentrated charge at the free end for singly clamped nanotube and finite kinematics, which accounts for large displacements, are investigated in details. We consider devices with $H \sim 0.1 \mu\text{m}$ in which the *van der Waals* force can be neglected

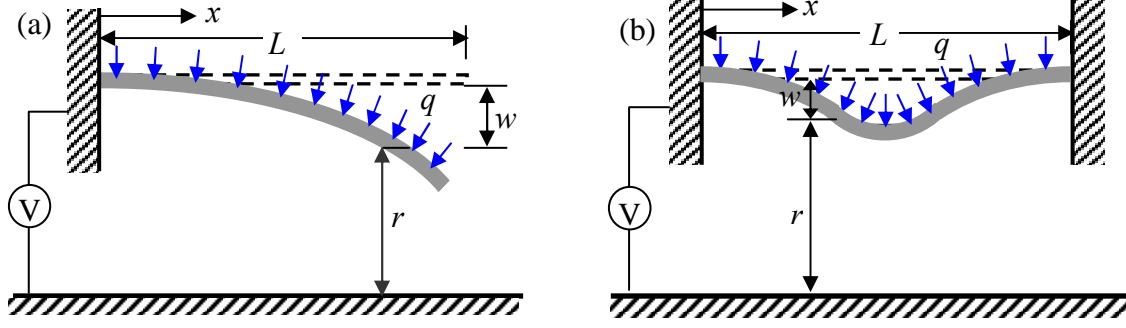


Fig. 1 Schematic of the finite kinematics configuration of a cantilever (a) and fixed-fixed (b) nanotube device subjected to electrostatic forces.

2. Modeling

The capacitance per unit length along the cantilever nanotube is approximated as⁵

$$C = C_d(r) \left\{ 1 + 0.85 [(H + R_{ext})^2 R_{ext}]^{1/3} \delta(x - x_{tip}) \right\} = C_d(r) \{1 + f_c\} \quad (1)$$

where the first term in the bracket accounts for the uniform charge along the side surface of the tube and the second term, f_c , accounts for the concentrated charge at the end of the tube (For clamped-clamped nanotubes, $f_c = 0$). $x = x_{tip} \neq L$, as a result of the finite kinematics. $\delta(x)$ is the Dirac distribution function. $C_d(r)$ is the distributed capacitance along the side surface per unit length for an infinitely-long tube, which is given by $C_d(r) = 2\pi\epsilon_0/a \cosh(1 + r/R_{ext})$ where r is the distance between the lower fiber of the nanotube and the substrate, and ϵ_0 is the permittivity of vacuum. Thus, the electrostatic force per unit length of the nanotube is given as follows:

$$q = \frac{1}{2} V^2 \frac{dC}{dr} = \frac{1}{2} V^2 \left(\frac{dC_d}{dr} \right) \{1 + f_c\} \quad (2)$$

If we just consider the bending of the singly clamped cantilever, the governing equation of the elastic line under finite kinematics is⁶

$$EI \frac{d^2}{dx^2} \left(\frac{d^2 w}{dx^2} \left(1 + \left(\frac{dw}{dx} \right)^2 \right)^{\frac{3}{2}} \right) = q \sqrt{1 + \left(\frac{dw}{dx} \right)^2} \quad (3)$$

where E is the Young Modulus, I is the moment of the inertia of the nanotube and w is the deflection of the nanotube. Eq. (3) clearly represents a more accurate description of the elastic behaviour of nanotubes than the more common equation assuming small

displacements, i.e. $EI \frac{d^4 w}{dx^4} = q$. For a doubly clamped nanotube, stretching becomes significant as a consequence of the rope-like behavior of a fixed-fixed nanotube subjected to finite kinematics. The elastic line equation becomes⁶,

$$EI \frac{d^4 w}{dx^4} - \frac{EA}{2L} \int_0^L \left(\frac{dw}{dx} \right)^2 dx \frac{d^2 w}{dx^2} = q \quad (4)$$

3. Result and discussion

Solving numerically the previous nonlinear equations for singly, and doubly clamped nanotube NEMS devices, respectively, the *pull-in* voltage corresponding to the nanotube collapsing onto the ground substrate can be predicted. The comparison between results numerically obtained and the results of analytically derived formulas⁷⁻⁸ obtained based on energy method is reported in Table 1.

Table 1: Comparison between pull-in voltages evaluated numerically and analytically for doubly (*D*) and singly (*S*) clamped nanotube devices, respectively. $E=1$ TPa, $R_{int}=0$. For cantilever nanotube device the symbol (w) denotes that the effect of charge concentration has been included.

Case	BC	H [nm]	L [nm]	$R=R_{ext}$ [nm]	V_{PI} [V] (theo. linear)	V_{PI} [V] (num. linear)	V_{PI} [V] (theo. non-linear)	V_{PI} [V] (num. non-linear)
1	<i>D</i>	100	4000	10	3.20	3.18	9.06	9.54
2	<i>D</i>	100	3000	10	5.69	5.66	16.14	16.95
3	<i>D</i>	200	3000	10	13.53	13.52	73.50	77.09
4	<i>D</i>	100	3000	20	19.21	18.74	31.57	32.16
5	<i>S</i>	100	500	10	27.28w)	27.05(w)	27.52(w)	27.41 (w)
6	<i>S</i>	100	500	10	27.28(w)	27.05(w)	30.87	31.66

It can be seen that the effect of finite kinematics is much significant for the doubly clamped boundary condition while for the singly clamped boundary condition, it is negligible. The effect of the concentrated charge for the singly clamped cantilever device is pronounced. The comparison between the numerical results and results of analytical close-form formula is in good agreement (with maximum discrepancy of 5 %).

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