

Analysis of Doubly Clamped Nanotube Devices in the Finite Deformation Regime

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In this paper, a nonlinear theory applicable to the design of nanotube based devices is presented. The role of finite kinematics for a doubly clamped nanotube device is investigated. In particular, we analyze the continuous deformation and instability (pull in) of a clamped-clamped nanotube suspended over an electrode from which a potential differential is imposed. The transformation of an applied voltage into a nanomechanical deformation indeed represents a key step toward the design of innovative nanodevices. Likewise, accurate prediction of pull-in/pull-out voltages is highly needed. We show that an energy-based method can be conveniently used to predict the structural behavior and instability corresponding to the ON/OFF states of the device at the so-called pull-in voltage. The analysis reveals that finite kinematics effects can result in a significant increase of the pull-in voltage. This increase results from a ropelike behavior of the nanotube as a consequence of the stretching imposed by the actuation.

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1 Introduction

Nanoelectromechanical systems (NEMS) are attracting much interest in the scientific community, since the discovery of nanotubes [1]. The first really true carbon-nanotube-based NEMS device, fully integrating electronic control and mechanical response, was developed only some months ago [2]. The authors reported the construction and successful operation of a fully synthetic nanoscale electromechanical actuator incorporating a rotatable metal plate, with a multi-walled carbon nanotube serving as the key motion-enabling element. Rueckes et al. [3] investigated a carbon nanotube-based nonvolatile random access memory by developing an innovative bistable nanoswitch based on electrostatic and van der Waals forces. The authors emphasized the extreme high integration level of the nanoswitches, approaching 10^{12} elements per square centimeter, and an element operation frequency in excess of 100 GHz. The viability of the concept was demonstrated by the experimental realization of a reversible bistable nanotube-based bit. In [4] the development of nanotweezers was reported. The mechanical capabilities of the nanotweezers were demonstrated by grasping and manipulating submicron clusters and nanowires.

In this context, the characterization of mechanical and electronic properties of nanotubes has been the subject of intense research. Their small size, low density, high stiffness, flexibility, and strength, as well as excellent electronic properties, suggest that nanotubes and nanowires are the most promising nanoscopic elements in the implementation of NEMS. For a recent review on the mechanics of carbon nanotubes the reader should refer to the paper by Qian et al. [5], and references therein. The strength of carbon nanotubes [6], was found to be of the order of 10–100 GPa. Furthermore, nanotubes (as well as nanoropes—composed

of several nanotubes—and nanowires—having differently shaped cross sections) possess an extremely high stiffness (Young's modulus of the order of 1 TPa [7,8]) and flexibility (strain at tensile failure of the order of 30% [9]). As a consequence of this large flexibility, the effect of the large displacements, usually neglected in analytical calculations, has to be considered in the analysis of NEMS.

In spite of the described fast acceleration in developing NEMS structures, key formulas needed in their design are still absent in the literature. The first extensive investigation of the behavior of nanotube-based devices has been recently reported [10]. In that paper, the differential equation of the elastic line of a nanotube suspended over an electrode and from which a differential in potential is imposed, was numerically solved according to continuum mechanics, assuming small displacements. The corresponding pull-in voltages, at the structural instability, were evaluated for different case studies. In addition, the first attempt to obtain an analytical formula for the pull-in voltage of the nanotube was also proposed, assuming for the nanotube a *platelike* undeformed shape, connected via a lumped stiffness to the ground electrode. As emphasized by the same authors, the proposed formula was not able to reproduce accurately all their numerical results.

In this paper we present a nonlinear energy-based theory for the prediction of the pull-in voltage of doubly clamped nanotubes under stretching. The equilibrium condition as well as the instability of the nanotube is obtained, respectively, by setting to zero the first and the second derivatives of the free energy of the system. A comparison between analytically predicted pull-in voltages and those obtained by numerically solving the corresponding governing equations is also provided.

2 Elastic Line Equation of the Nanotube Under Finite Kinematics

In this section we derive, in the finite deformation regime, the elastic line equation for a nanotube. We focus the attention on a doubly clamped nanotube suspended over an electrode at a distance $r=H$ from which a difference V in the electrostatic potential is imposed (nanoswitch) which is schematically shown in Fig. 1. Note that this is equivalent to the problem of two identical doubly clamped nanotubes placed at distance $2r=2H$ under a difference in voltage $2V$, as imposed by the symmetry.

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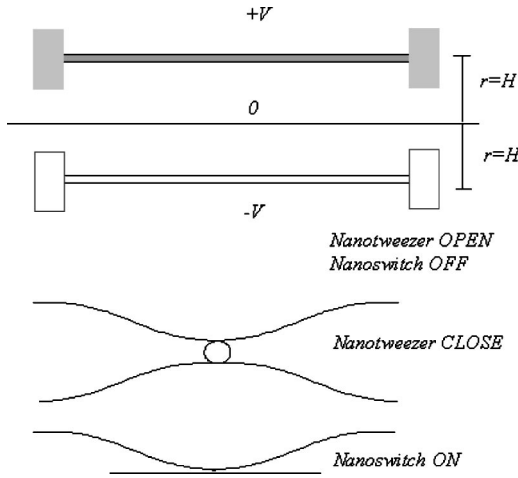


Fig. 1 Schematics of doubly clamped nanotube based nanoswitches and nanotweezers

The electrostatic and van der Waals energies per unit length can be evaluated by the following relationships [10]:

$$\frac{dE_{\text{elec}}}{dz} = \frac{\pi\epsilon_0 V^2}{\cosh^{-1}\left(1 + \frac{r}{R}\right)},$$

$$\frac{dE_{\text{vdW}}}{dz} = \sum_{R=R_{\text{int}}}^{R_{\text{ext}}} \sum_{r=r_{\text{int}}}^{r_{\text{int}}+(N_G-1)d} \frac{\pi^2 C_6 n^2 d^2 R(r+R)[3R^2 + 2(r+R)^2]}{2[(r+R)^2 - R^2]^{7/2}}, \quad (1)$$

where z is the axial coordinate of the cantilever nanotube, R_{int} and $R \equiv R_{\text{ext}}$ are the inner and outer radius of a multiwalled nanotube, N_G is the number of layers in the substrate (graphene), d is the interlayer distance (for graphite $d=0.335$ nm). In addition, $r \equiv r_{\text{int}}$ is the gap between the nanotube (external wall) and the surface layer of the substrate, where n is the atomic density, that for graphite is equal to $n=1.14 \times 10^{29} \text{ m}^{-3}$, and $\epsilon_0=8.85 \times 10^{-12} \text{ C}^2 \text{ N}^{-1} \text{ m}^{-2}$ is the vacuum permittivity.

The corresponding forces per unit length q_{elec} and q_{vdW} can be evaluated, according to Eq. (1) as

$$q_{\text{elec}} = -\frac{d(dE_{\text{elec}}/dz)}{dr}, \quad q_{\text{vdW}} = -\frac{d(dE_{\text{vdW}}/dz)}{dr}. \quad (2)$$

Based on continuum mechanics, the quasistatic structural behavior of the nanotube, can be obtained solving the elastic line equation, namely,

$$EI \frac{d^4 w}{dz^4} = q_{\text{vdW}} + q_{\text{elec}}, \quad I = \frac{\pi(R_{\text{ext}}^4 - R_{\text{int}}^4)}{4}, \quad (3)$$

where $w(z)=H-r(z)$ is the nanotube deflection, H is the nominal gap between nanotube and electrode, and E is the Young's modulus of the nanotube, with moment of inertia I .

It is important to underline that Eq. (3) assumes small displacements. On the other hand, due to the large flexibility of the nanotube, the role of the finite kinematics (large displacements) could become relevant. According to these considerations, we have to consider the complete expression for the elastic curvature. In addition, it is important to note that large deformations could imply, for doubly clamped nanotubes, also the stretching of the element. Finally, under large deformations, the electrostatic forces, orthogonal to the surface of the nanotube, have to be considered with respect to the deformed configuration (we neglect the effect of the finite kinematics on the Lennard-Jones forces per unit length, i.e., van der Waals and Pauli forces, which become signifi-

cant only for very small gaps, i.e., few nanometers). In the dynamic regime, the damping and inertia forces must be also added (e.g., to consider variable applied voltages, thermal vibrations, free vibrations, and so on). According to these considerations, the complete expression of the elastic line equation for a nanotube device is

$$EI \frac{\partial^2}{\partial z^2} \left(\frac{\frac{\partial^2 w}{\partial z^2}}{\left[1 + \left(\frac{\partial w}{\partial z}\right)^2\right]^{3/2}} \right) - \frac{EA}{2L} \int_0^L \left(\frac{\partial w}{\partial z}\right)^2 dz \frac{\frac{\partial^2 w}{\partial z^2}}{\left[1 + \left(\frac{\partial w}{\partial z}\right)^2\right]^{3/2}} = q_{\text{vdW}} + q_P + \left(q_{\text{elec}} - \gamma \frac{\partial w}{\partial t} - \mu \frac{\partial^2 w}{\partial t^2} \right) \left[1 + \left(\frac{\partial w}{\partial z}\right)^2\right]^{1/2}, \quad (4)$$

where μ and γ represent the mass and the damping per unit length of the nanotube and t is the time. The Pauli force per unit length q_P is obtained from the repulsive part of the Lennard-Jones potential [10]. From the Q -factor of the nanotube (between 170–500 [11]), $\gamma = \mu \omega_0 / Q$, where ω_0 is its fundamental rotating frequency. The term $\left[1 + \left(\frac{\partial w}{\partial z}\right)^2\right]^{3/2}$ represents the correction for the curvature, that must be considered under large displacements. The term $\cos \vartheta = (1 + (\partial w / \partial z)^2)^{-1/2}$ has to be introduced to consider the changing in the positions of the loads that remain perpendicular to the nanotube axis, as a consequence of the large displacements, involving not necessarily small rotations of the cross-section by an angle ϑ . For a clamped-clamped nanotube the axial force is equal to $N(w) = EA / 2L \int_0^L (\partial w / \partial z)^2 dz$.

Some interesting results were obtained [10] by solving numerically Eq. (3). The more general Eq. (4) was also solved numerically [12,13]. On the other hand, here we prefer obtaining an analytical solution under simplified hypotheses for the pull-in voltage, corresponding to the quasistatic collapse of the nanotube, i.e., assuming $\gamma = \mu = 0$. Instead of solving Eq. (4) in an approximate way, we will obtain the equilibrium and the instability of the nanosystem by minimizing the free energy and its first derivative.

3 Small Deformation

We consider a clamped-clamped nanotube of length L . For the small deflection case of a clamped-clamped nanotube loaded by a constant force per unit length, we assume a function $w(z)$ satisfying the boundary conditions $w(z=0, L) = w'(z=0, L) = 0$, namely,

$$w(z) \approx 16 \left[\left(\frac{z}{L}\right)^2 - 2\left(\frac{z}{L}\right)^3 + \left(\frac{z}{L}\right)^4 \right] c, \quad (5)$$

where $w(z=L/2)=c$ is here an unknown constant that represents the displacement of the central point.

As a consequence, the elastic energy, assuming small displacements, as well as the electrostatic and van der Waals energies stored in the nanotube can be obtained by integration as

$$E_{\text{elast}}(c) = \frac{EI}{2} \int_0^L \left(\frac{d^2 w}{dz^2}\right)^2 dz, \quad (6a)$$

$$E_{\text{elec}}(c) \approx \int_0^L \frac{dE_{\text{elec, vdW, P}}\{r[w(z)]\}}{dz} dz. \quad (6b)$$

We investigate the validity of the form of Eq. (5) by evaluating the associated fundamental frequency and by comparing it with the well-known value for a clamped-clamped nanotube. Equating the maximum values of the elastic strain energy of Eq. (6a) and of the kinetic energy $K(t) = 1/2 \int_0^L (dw/dt)^2 \mu dz$, with μ mass per unit length of the nanotube, during its free-vibration with $w(z, t) \approx w(z) \sin \omega_0 t$, one finds the estimation of the fundamental frequency ω_0 of the nanotube. The ratio between the estimated fundamental frequency and the real one is found to be close to 1. We conclude that the form of Eq. (5) is good for our scope.

The free-energy (or total potential energy) of the system can be written as

$$W(c) = E_{\text{elast}}(c) - E_{\text{elec}}(c) - E_{\text{vdW}}(c) - E_{\text{p}}(c). \quad (7a)$$

Equilibrium and stability are obtained from

$$\frac{dW(c)}{dc} = 0, \quad (7b)$$

$$\frac{d^2W(c)}{dc^2} = 0. \quad (7c)$$

The equilibrium condition is reached when the free-energy reaches a minimum value (Eq. (7b)). On the other hand, the structural instability occurs at the so-called pull-in voltage, when the second order of the free-energy becomes zero (Eq. (7c)). According to [10], the effects of the van der Waals and Pauli forces for these boundary conditions is negligible, even for small gaps; hence, we take $E_{\text{vdW,p}} \approx 0$.

The electrostatic energy per unit length can be approximated as

$$\begin{aligned} \frac{dE_{\text{elec}}}{dz} &\approx \frac{\pi\epsilon_0 V^2}{\ln\left(\frac{2(R+H-w)}{R}\right)} = \frac{\pi\epsilon_0 V^2}{\ln\left(\frac{2(H+R)}{R}\right)} \\ &\times \left[1 + \sum_{i=1}^{\infty} \left(\frac{1}{\ln\left(\frac{2(H+R)}{R}\right)} \sum_{j=i}^{\infty} \frac{1}{i} \left(\frac{w}{(H+R)}\right)^j \right)^i \right]. \quad (8) \end{aligned}$$

Employing Eq. (6b), the total electrostatic energy can be expressed as

$$\begin{aligned} E_{\text{elec}}(c) &= \frac{\pi\epsilon_0 V^2 L}{\ln\left(\frac{2(H+R)}{R}\right)} \\ &\times \left[1 + \sum_{i=1}^{\infty} \left(\left[\frac{1}{\ln\left(\frac{2(H+R)}{R}\right)} \right]^i \sum_{j=i}^{\infty} a_{ij} \left(\frac{c}{(H+R)}\right)^j \right) \right], \quad (9) \end{aligned}$$

where $\{a_{ij}\}$ are constants. Let $S(c) = \sum_{i=1}^{\infty} \left(\left[\frac{1}{\ln\left(\frac{2(H+R)}{R}\right)} \right]^i \sum_{j=i}^{\infty} a_{ij} \left(\frac{c}{(H+R)}\right)^j \right)$.

From Eqs. (5) and (6a), the total elastic energy of the nanotube can be obtained as

$$E_{\text{elast}} = \frac{512 EI}{5 L^3} c^2. \quad (10)$$

From Eqs. (7a) and (7b), the equilibrium condition provides

$$V(c) = \frac{H+R}{L^2} \ln\left(\frac{2(H+R)}{R}\right) \sqrt{\frac{1024 EI}{5 \pi \epsilon_0 S'(c)} \left(\frac{c}{H+R}\right)}. \quad (11)$$

The central displacement of the nanotube at pull-in c_{PI} can be obtained from

$$\frac{dV(c)}{dc} = 0, \quad (12)$$

which means the pull-in corresponds to a maximum in V . Hence, the pull-in voltage can be written as

$$V_{\text{PI}} = k \frac{H+R}{L^2} \ln\left(\frac{2(H+R)}{R}\right) \sqrt{\frac{EI}{\epsilon_0}}, \quad (13)$$

where $k = \frac{1024}{5 \pi S'(c_{\text{PI}})} \left(\frac{c_{\text{PI}}}{H+R}\right)$.

4 Finite Kinematics

To take into account the nonlinear effect arising from finite kinematics, we have to evaluate the energy stored in the beam not

only due to bending but also due to stretching. This represents the predominant effect of the finite kinematics for the doubly clamped nanotube.

The strain due to bending is

$$\epsilon_b = -y \frac{d^2 w}{dz^2}, \quad (14)$$

where y has the origin in the centroid of the cross section, and is parallel to the direction of the loads. In addition, the mean value of stretching due to the displacement w , noting that $ds^2 = dz^2 + dw^2$, is [14]

$$\epsilon_s = \frac{ds - dz}{ds} \approx \frac{1}{2L} \int_0^L \left(\frac{dw}{dz}\right)^2 dz. \quad (15)$$

As a consequence, the elastic energy stored in the nanotube, is

$$E_{\text{elast}} = \frac{E}{2} \int_A \int_0^L (\epsilon_s + \epsilon_b)^2 dA dz, \quad (16)$$

where $A = \pi(R_{\text{ext}}^2 - R_{\text{int}}^2)$ is the cross-section area of the nanotube. Considering Eq. (5), the result is

$$E_{\text{elast}} = \frac{512 EI}{5 L^3} c^2 \left(1 + \frac{128 c^2}{3003 \rho^2} \right), \quad (17)$$

where the radius of inertia ρ is defined as $I = A\rho^2$. The first term corresponds to the bending, whereas the second nonlinear term represents the elastic strain energy stored in the beam due to the stretching of the nanotube. Note that the force (derivative of the energy) due to bending is linear, while the one due to stretching is cubic.

Considering the energy as the fundamental quantity to derive a nonlinear correction for the stretching, we have to consider the increase in beam stiffness as

$$EI \rightarrow \left(1 + \frac{128 c^2}{3003 \rho^2} \right) EI. \quad (18)$$

Therefore, the equilibrium condition gives

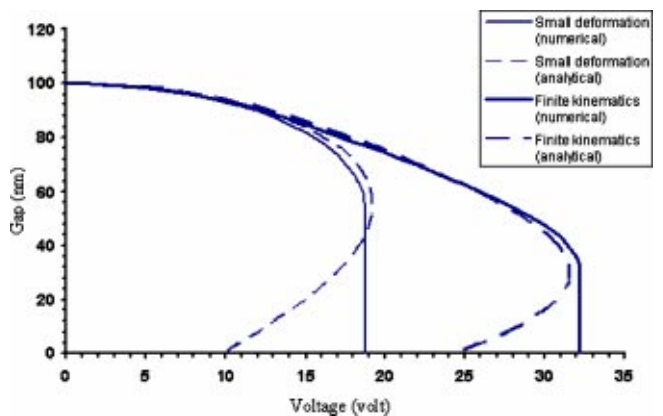


Fig. 2 Comparison between analytical predictions and numerical results. Plot of applied voltage versus gap for both small deformation and finite kinematics. The gap is measured between the axis of the nanotube and the electrode in the middle of the span.

Table 1 Comparison between pull-in voltages evaluated numerically and analytically by Eqs. (13) and (20) for doubly clamped nanotube devices, respectively. $E=1.0$ TPa, $R_{\text{int}}=0$. SD refers to small deformation, FK refers to finite kinematics.

Case	H [nm]	L [nm]	$R=R_{\text{ext}}$ [nm]	V_{PI} [V] (theo-SD)	V_{PI} [V] (num-SD)	V_{PI} [V] (theo-FK)	V_{PI} [V] (num-FK)
1	100	4000	10	3.20	3.18	9.06	9.54
2	100	3000	10	5.69	5.66	16.14	16.95
3	100	2000	10	12.81	12.73	36.31	38.14
4	150	3000	10	9.45	9.43	38.93	40.92
5	200	3000	10	13.53	13.52	73.50	77.09
6	100	3000	20	19.21	18.74	31.57	32.16
7	100	3000	30	38.57	37.72	51.96	50.63

$$V^{\text{FK}}(c) = V(c) \sqrt{\left(1 + \frac{128}{3003} \left(\frac{c}{\rho}\right)^2\right)} = \frac{H+R}{L^2} \ln\left(\frac{2(H+R)}{R}\right) \times \sqrt{\frac{1024EI \left[1 + \frac{128}{3003} \left(\frac{c}{\rho}\right)^2\right] \left(\frac{c}{H+R}\right)}{5\pi\epsilon_0 S'(c)}}. \quad (19)$$

Stationary condition, Eq. (12), applied to V^{FK} (FK refers to finite kinematics), provides the value of c at pull in. The pull-in voltage can then be expressed as

$$V_{\text{PI}}^{\text{FK}} = k^{\text{FK}} \frac{H+R}{L^2} \ln\left(\frac{2(H+R)}{R}\right) \sqrt{\frac{EI}{\epsilon_0}}, \quad (20)$$

where $k^{\text{FK}} = \sqrt{\frac{1024}{5\pi S'(c_{\text{PI}})} \left(\frac{c_{\text{PI}}}{H+R}\right) \left[1 + \frac{128}{3003} \left(\frac{c_{\text{PI}}}{\rho}\right)^2\right]}$.

5 Comparison Between Analytical Prediction and Numerical Simulations

An assessment of the derived analytical formulas is performed by comparing the results obtained solving numerically the corresponding elastic line equations, for both small deformation (only bending) and finite kinematics (bending+stretching). The nanotube properties and dimensions used here are Young's modulus $E=1.0$ TPa, $R_{\text{ext}}=20$ nm, $R_{\text{int}}=0$ nm, and $L=3000$ nm. The initial gap $H=100$ nm is also employed. Note that the theory does not involve a best fit parameter. The detailed comparison is reported in Fig. 2. In this figure, the applied voltage versus the gap, in the middle of the span between the nanotube and the electrode, is theoretically evaluated and plotted for both the small deformation model Eq. (11) and the finite kinematics model Eq. (19). These plots are compared in the same figure with the small deformation and finite kinematics numerical results obtained by solving Eq. (3) using a finite difference scheme. When evaluating the analytical solution, $i=1$ to 4 and $j=1$ to 10 are employed in the series of Eq. (8). The corresponding constants $\{a_{ij}\}$ in Eq. (9) are obtained using Mathematica®. From Fig. 2, it is clear that the finite kinematics effect is indistinguishable when the deformation is small and it gradually becomes significant with the increase in deformation. It is noted that the theoretical prediction curve can be divided into two parts with the separation point at $V=V_{\text{PI}}$ and $c=c_{\text{PI}}$. The part that corresponds to $c \leq c_{\text{PI}}$ follows the numerical results and can be experimentally implemented. The part that corresponds to $c > c_{\text{PI}}$ could be experimentally captured only by a displacement-control device. On the other hand, if the NEMS is voltage controlled, it will follow the unstable path (at $V=V_{\text{PI}}$) until reaching the contact. The difference between the two paths is related to the kinetic energy released by the structure after pull in when the device is actuated under voltage control. From Fig. 2, it can be concluded that the analytical results are in excellent agreement with the numerical results.

The effects of the geometry of the nanotube L and R and the step height H on the pull-in voltage of the NEMS device have also been examined both analytically and numerically. The results are reported in Table 1. Columns five and six in Table 1 compare analytical and numerical pull-in voltage predictions under the as-

sumption of small deformations. Columns seven and eight in Table 1 compare analytical and numerical pull-in voltage predictions under the assumption of finite kinematics. The agreement between the analytical predictions and numerical results is satisfactory (with a maximum discrepancy of 5%).

Note that an oversimplified model, e.g., assuming a capacitance of two parallel plates and a concentrated stiffness [10], can result in significant errors in the evaluation of the pull-in voltage. The importance of a more accurate model, that is the aim of this paper, has been recently emphasized in [4] where, by assuming a parallel plate capacitance, a pull-in voltage of 9.4 V was predicted in contrast to the experimental measurement of 8.5 V.

6 Closure

We have presented a theory to analyze nanotube structures, which is particularly suited to the design of NEMS and nanosensors. Comparison with numerical results shows good agreement. The formulas here reported could represent a considerable step forward in the understanding and development of nanosensors and NEMS. Note that the analysis is also applicable to microelectromechanical systems (MEMS).

With improvements in nanomanipulation and manufacturing of nanodevices we hope experimental measurements will become available, which will confirm or identify limitations of the theoretical predictions here reported.

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