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Non-linear dynamics of nanotube based NEMS

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Abstract

In this paper the non-linear dynamics of nanotubes is investigated with a look into their applications in nanoelectromechanical systems (NEMS). The understanding of the dynamics of NEMS, always oscillating -at least as a consequence of the thermal vibrations- represents a still open and fundamental issue towards an optimal dynamic design of nanotube based devices. The vibrations of NEMS are usually studied assuming a linear behavior and without considering the effect of the electrical field imposed to control the device. In spite of this, the presence of the electrostatic charges implies that the nanotube cannot be considered as free, as usually assumed. Moreover, linear behavior, implicitly corresponding to assume small displacements, seems to be in contrast with the observed high flexibility of nanotubes, capable of undergoing large displacements remaining in elastic regime. In this paper, we try to remove these assumptions, deriving the corresponding equation

governing the motion of the device under large displacements and electrostatic loading. The role of the van der Waals forces, significant only for very small gaps (few nanometers), is also investigated. Instead of solving numerically the derived equation for different case studies, we obtain an approximated solution studying the oscillations around the static configuration that minimizes the free-energy of the NEMS. Finally, the amplitude of the intrinsic oscillations at 0K, as imposed by the uncertainty principle, are estimated. A validation of the analysis is achieved by a comparison with experimental observations of thermal oscillations in singly or doubly clamped nanotubes. In addition, the intensity of the electrical field corresponding to a vanishing oscillating frequency, i.e., to a structural instability, is predicted and compared with numerical simulations. Such simple prediction of the pull-in voltage is shown to be fundamental, since it represents the key design parameter, describing the on/off transition of the device.

1. Introduction

Nanoelectromechanical systems (NEMS) seem to have the capability of revolutionizing the electronic components of the future. Their tremendous miniaturized size and high fundamental frequency would result in a density of the order of 10^{12} elements over square centimeter and operation frequency in the EHF band (Extra High Frequency, 30-300GHz). Due to their extreme electromechanical properties, nanotubes represent the ideal candidate for such applications. A nanotube based NEMS (e.g., nanoswitch, nanotweezers...) can be thought as a singly or doubly clamped nanotube suspended at a given gap over an electrode, from which a differential in the electrostatic potential is imposed. Increasing the voltage, a structural instability of the nanotube, corresponding to the on/off states of the device will take place at the so-called pull-in voltage.

Ever since their discovery [1], nanotubes have attracted a major interest in the scientific community. In the last decade, the mechanical and electronic properties of nanotubes have been investigated. Small size, low density, high stiffness, flexibility and strength, as well as excellent electronic properties, suggest that nanotubes have the potential to impact the development of novel composites, electronic devices and NEMS. Nanotubes (as well as nanoropes -composed by several nanotubes- and nanowires – having different shaped compact cross-sections) are envisioned as the ultimate fiber reinforcements as a consequence of their extremely high stiffness (Young's modulus of the order of 1TPa [2,3]) and flexibility (strain at tensile failure of the order of 30%, [4]). Their strength, investigated in [5], is of the order of 10-100GPa. For a detailed review on the mechanics of carbon nanotubes the reader should refer to [6].

Recently, some research groups have been able to manufacture NEMS devices. For instance, Kim and Lieber [7] developed a nanotweezers. The mechanical capabilities of the nanotweezers were demonstrated by gripping and manipulating submicron clusters and nanowires. Likewise, Rueckes et al. [8] investigated a carbon nanotube-based nonvolatile random access memory, by considering an innovative bistable nanoswitch based on electrostatic and van der Waals forces. The viability of the concept was demonstrated by the experimental realization of a reversible bistable nanotube-based bit. Furthermore, the first really true nanotube-based NEMS, fully integrating electronic control and mechanical response, was developed only some months ago by Fennimore et al. [9] by realization of a rotational motor. The authors reported the construction and

successful operation of a fully synthetic nanoscale electromechanical motor incorporating a rotational metal plate with a multi-walled carbon nanotube serving as the key motion-enabling element.

In spite of this fast acceleration in the development of NEMS structures, key analyses in the static and dynamic design of NEMS are still absent in literature. The first extensive static investigation of the behavior of NEMS devices has been reported by Dequesnes et al. [10]. In that paper, the linearized equation of the elastic line of a nanotube suspended over an electrode and from which a differential electrical 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 cases. 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 plate-like undeformed shape, connected via a lumped stiffness to the ground electrode. As emphasized by the same authors, the proposed formula was not able to accurately reproduce all their numerical results.

In this paper we present a free-energy based theory for the prediction of the (non-linear) dynamics of nanotube based NEMS. A validation of the model is achieved by setting to zero the frequency of the system, to predict the mechanical instability corresponding to the pull-in of the device. The results are compared with numerical simulations, showing a good correspondence.

An additional validation of the analysis is achieved by a comparison with experimental observations of thermal oscillations in singly or doubly clamped nanotubes. The amplitude of the oscillations at 0K, as imposed by the uncertainty principle, is also estimated.

2. Non-linear elastic line equation

Let us focus the attention on a singly or doubly clamped nanotube suspended over an electrode at a distance H from which a difference, V , in the electrostatic potential is imposed, under a given temperature T (Fig. 1).

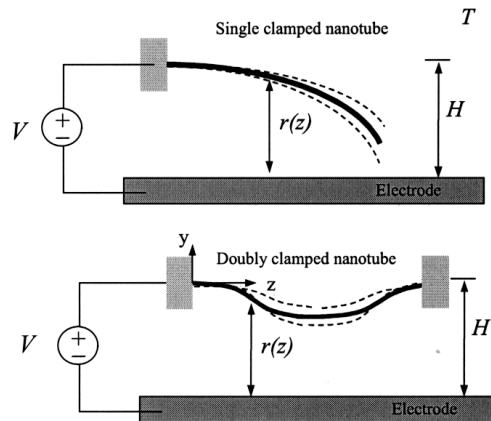


Figure 1. Singly and doubly clamped nanotube devices at a given temperature T .

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

$$\frac{dE_{elec}}{ds} = \frac{\pi\epsilon_0 V^2}{\cosh^{-1}\left(1 + \frac{r}{R}\right)} \quad (1a)$$

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

where s is the natural axial co-ordinate along the deflected nanotube (coincident with the horizontal co-ordinate z only for small displacements), R_{int} and $R \equiv R_{ext}$ are the inner and outer radius of a (multi-walled) nanotube, N_G is the number of layers in the substrate (usually graphene), d is the interlayer distance (for graphited $d = 0.335\text{nm}$). In addition, $r \equiv r_{int}$ is the gap between the nanotube (external wall) and the surface layer of the substrate, where n is the atomic density (for graphite is equal to $n = 1.14 \times 10^{29} \text{m}^{-3}$); $\epsilon_0 = 8.85 \times 10^{-12} \text{C}^2 \text{N}^{-1} \text{m}^{-2}$ is the vacuum permittivity and C_6 is a material constant (for graphite is equal to $C_6 = 2.43 \times 10^{-78} \text{Nm}^7$).

The corresponding forces q_{elec} and q_{vdW} per unit length acting on the nanotube can be evaluated by derivation:

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

Based on continuum mechanics, the linear ($s=z$) quasi-static structural behavior of the nanotube can be obtained solving the classical elastic line equation, namely:

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

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

It is important to understand 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 by an axial force $N(w)$. Finally, under large displacements, the electrostatic forces, orthogonal to the surface of the nanotube, have to be considered with respect to the deformed configuration (here we assume the same consideration for the van der Waals forces). In the dynamic regime, the damping and inertia forces must be also added (e.g., to consider variable electrical fields, thermal vibrations, free vibrations, etc.). According to these considerations, the complete expression of the elastic line equation has to be written as:

$$EI \frac{\partial^2}{\partial z^2} \left(\frac{\frac{\partial^2 w}{\partial z^2}}{\left[1 + \left(\frac{\partial w}{\partial z}\right)^2\right]^{\frac{3}{2}}} \right) - N \left(\frac{\frac{\partial^2 w}{\partial z^2}}{\left[1 + \left(\frac{\partial w}{\partial z}\right)^2\right]^{\frac{3}{2}}} \right) = \left(q_{elec} + q_{vdw} - \gamma \frac{\partial w}{\partial t} - \mu \frac{\partial^2 w}{\partial t^2} \right) \left(1 + \left(\frac{\partial w}{\partial z}\right)^2 \right)^{\frac{1}{2}} \quad (4)$$

where μ and γ represent the mass and the damping per unit length of the nanotube and t is the time. The Pauli's force per unit length, q_p , has to be added for gap smaller than ~ 1 nm and could be obtained from the repulsive part of the Lennard-Jones potential [11] as done for the van der Waals forces. From the Q-factor of the nanotube (of the order of 200-500 [12]), $\gamma = \mu\omega/Q$ where ω is its fundamental (rotating) frequency. The term

$\left[1 + \left(\frac{\partial w}{\partial z}\right)^2\right]^{\frac{3}{2}}$ represents the correction for the curvature, that must be considered under

large displacements. The term $\cos \vartheta = \left(1 + \left(\frac{\partial w}{\partial z}\right)^2\right)^{-\frac{1}{2}}$ has to be introduced to consider the

change in the positions of the loads that remain perpendicular to the nanotube axis, as a consequence of the large displacements, involving a finite rotation ϑ of the cross-

section. For a nanotube, of cross-section area A and length L , $N \approx \frac{EA}{2L} \int_0^L \left(\frac{\partial w}{\partial z}\right)^2 dz$ if

clamped-clamped or $N = 0$ if cantilever. Note that for moderately large displacements

$$\left(\frac{\partial w}{\partial z}\right)^2 \ll 1.$$

Some interesting results were obtained [10], solving numerically the static linear eq. (3). The more general dynamic non-linear eq. (4) could also be solved numerically. Instead of solving eq. (4) in an approximated way, we will study the dynamics of the nanotube by a free-energy approach. As a consequence of the high value of the Q-factor we neglect the damping of the NEMS.

3. Vibrations around large deformed configurations

The aim of this section is the estimation of the NEMS oscillations around a deformed configuration due to the electrostatic and van der Waals forces.

Let us consider a deformed static configuration w_S assumed as a given arbitrary function satisfying the boundary conditions, with one (or more) unknown free parameter c_S (e.g., $w_S \approx c_S s^2/L^2$ for cantilever), indicating the maximum displacement of the nanotube (of the tip for cantilever or of the middle point for a clamped-clamped nanotube). The oscillations around this configuration can be described by:

$$w(s,t) = w_S(s) + w_D(s,t) \quad (5)$$

For the fundamental frequency:

$$w_D(s,t) \approx \frac{w_S(s)}{c_S} c_D \sin(\omega t) \quad (6)$$

where c_D represents the maximum amplitude of the harmonic oscillations around the equilibrium position described by c_S . Accordingly, the kinetic energy of the system will be:

$$K(t) = \frac{1}{2} \int_M \left(\frac{dw(s,t)}{dt} \right)^2 dM = \frac{\mu}{2} \int_0^L \left(\frac{dw_D(s,t)}{dt} \right)^2 ds \quad (7)$$

where M is the mass of the nanotube, and $\mu = \rho_m A$, with A cross-section area and ρ_m density (for carbon $\rho_m = 2260 \text{Kg/m}^3$). Eq. (7) can be rewritten as:

$$K(t) = \frac{1}{2} m_{eq} c_D^2 \omega^2 \cos^2(\omega t), \quad m_{eq} = \alpha M \quad (8)$$

where α is dependent on the chosen form for w_S (e.g., rough forms of w_S give estimations for cantilever of $\alpha \approx 1/5$ and for clamped-clamped of $\alpha \approx 13/35$, [13]) and can be derived by comparing eqs. (7) and (8).

In comparison, indicating the free-energy of the NEMS by $W(c)$, where $c = c_S + c_D \sin(\omega t)$, and fixing its reference by imposing $W(c_S) = 0$, equating the maximum value of the free-energy and the maximum kinetic energy of the nanotube, gives the estimation of the fundamental frequency ω as:

$$\omega^2 = \frac{2W_{\max}}{m_{eq} c_D^2} \quad (9)$$

If the kinetic energy (e.g., its mean value) is a given quantity, from eq. (8) and (9), the frequency and the amplitude of the oscillations can be derived. Note that in general (if the oscillations are large) the frequency ω will be a function also of the amplitude c_D , as described by eq. (9), showing a non-linear behaviour. For small oscillations, the frequency becomes amplitude-independent as emphasized in the next section.

3.1 Small oscillations

If the oscillations are small (also around a large deflected configuration) we can develop the free energy in series. Since at the static equilibrium the free-energy must present a minimum, i.e., $\left. \frac{dW(c)}{dc} \right|_{c=c_S} = 0$, as well as $W(c_S) = 0$ (according to the chosen reference system), we have:

$$W(c) \cong \frac{1}{2} \left. \frac{d^2W(c)}{dc^2} \right|_{c=c_S} (c - c_S)^2 = \frac{1}{2} \left. \frac{d^2W(c)}{dc^2} \right|_{c=c_S} (c_D \sin(\omega t))^2 \quad (10)$$

so that, applying eq. (9), it follows:

$$\omega^2 = \frac{\left. \frac{d^2 W(c)}{dc^2} \right|_{c=c_S}}{m_{eq}} \quad (11)$$

Note that, under these assumptions, ω does not depend on the amplitude c_D but only on the external fields (e.g., the electrical one), included in the free-energy term.

3.1.1 Free-oscillations

Focusing the attention on the free-oscillations, the free-energy becomes coincident with the elastic energy stored in the nanotube, i.e., $W(c) = E_{elast}(c)$, where:

$$E_{elast}(c) = \frac{EI}{2} \int_0^L \left(\frac{d\vartheta}{ds} \right)^2 ds = \frac{\beta EI}{L^3} c^2 \quad (12)$$

where ϑ defines the slope of the elastic line of the nanotube, i.e., $\vartheta = dw/dz$, and β is dependent on the chosen form for w_S (e.g., rough estimations are for cantilever $\beta \approx 1$ and for clamped-clamped $\beta \approx 48$, [13]). Thus, from eq. (11):

$$\omega^2 = \frac{2\beta EI}{L^3 m_{eq}} \quad (13)$$

3.1.2 Thermal vibrations

For thermal vibrations at absolute temperature T , the Equipartition Theorem implies a known mean value $k_B T/2$ (k_B is the Boltzmann's constant) of the kinetic energy associated to each degree of freedom, hence:

$$\langle K(\tau) \rangle = \frac{1}{P} \int_P K(\tau) d\tau = \frac{k_B T}{2} \quad (14)$$

where $P = 2\pi/\omega$ is the period of the oscillation. By comparing eq. (14) with the mean value of eq. (8), in the light of eq. (11), gives:

$$c_D^2 = \frac{2k_B T}{\left. \frac{d^2 W(c)}{dc^2} \right|_{c=c_S}} \quad (15)$$

from which we can obtain the amplitude c_D of the thermal vibration around the position described by c_S . The frequency is given by eq. (11).

The Equipartition Theorem applied to the higher modes m fixes their relative amplitudes, that falls off as $\sim 1/m^2$. Thus, the first mode ($m=1$, that we are investigating) is clearly the predominant one. Note that at room temperature, the higher modes with frequencies ω_m become unimportant well before that their quantum accessibility comes into question, i.e., when $k_B T_{room} \approx \hbar \omega_m$, ($\hbar = h/(2\pi)$, with h Planck's constant),

corresponding to m of the order of 85 [3]. At zero temperature, the quantum effect becomes predominant, as we will emphasize in Section 3.2.

3.1.3 Free-thermal vibrations

Considering the thermal vibrations around the relaxed configuration $W(c) = E_{elast}(c)$, and introducing eq. (12) into eq. (15) yields:

$$c_D^2 = \frac{L^3 k_B T}{\beta EI} \quad (16)$$

with ω given by eq. (13).

3.1.4 Instability

The instability of the system, arising at the so called pull-in voltage, is achieved when the global stiffness of the NEMS becomes negligible, i.e., when the frequency of the oscillations formally goes to zero:

$$\omega^2 = \frac{d^2 W(c)}{dc^2} \Big|_{c=c_S} = 0 \quad (17)$$

According to eqs. (11) and (15) the thermal vibrations are predicted to be infinitely large at zero frequency. Practically, when they become large enough, the approximation of small vibrations is not more valid and the amplitude will be limited. From the condition of eq. (17), the pull-in voltage can be estimated.

The kinetic energy released after the pull-in can be evaluated as:

$$K_{PI} \cong W_{PI} - W_{contact} \quad (18)$$

where W_{PI} is the free-energy at the pull-in and $W_{contact}$ is the free-energy in the collapsed configuration.

3.2 The oscillations at 0K

The Hamiltonian of the NEMS can be written as ($W(c_S)=0$):

$$H(c,t) = K(c,t) + W(c) \quad (19)$$

The Schrödinger's equation of the continuum system can be correspondingly written in a simple manner, as a consequence of the reduction to one degree of freedom, as:

$$\left(-\frac{\hbar^2}{2m_{eq}} \frac{d^2}{dc^2} + W(c) \right) \psi_n(c) = E_n \psi_n(c) \quad (20)$$

where E_n are the energy eigenvalues and ψ_n are the eigenfunctions describing the fundamental vibrational states. Eq. (20) can be solved numerically. For small dynamic displacements around a (large) deflected configuration we can substitute the conditions of eqs. (10) and (11), finding the well-known discrete quantized energy levels of the harmonic oscillator:

$$E_n \approx \left(\frac{1}{2} + n\right) \hbar \omega \quad (21)$$

note that here ω is not the fundamental frequency of the cantilever nanotube, but, according to eq. (11), takes into account the external fields included in the free-energy. Obviously, the lowest energy level is predicted to be different from zero also at zero temperature:

$$E_0 \approx \frac{\hbar \omega}{2} \quad (22)$$

as imposed by the Heisenberg's Principle (the total energy is the sum of the potential and kinetic energy, both positively defined; considering $E_0 \approx 0$ would imply that both position and velocity of the system are known (and equal to zero), in contrast with the uncertainty principle). Between two adjacent levels the energy gap is obviously $\Delta E = E_{n+1} - E_n = \hbar \omega$.

The condition for which eq. (22) equals eq. (14) corresponds to the temperature for which the "vibrations" (corresponding to the borderline with the quantum accessibility) at the zero point become larger than the thermal vibrations:

$$k_B T \approx \hbar \omega \quad (23)$$

Substituting eq. (23) into eq. (15) implies considering the energy of eq. (22) as the mean value of the kinetic energy at zero Kelvin, thus the amplitude of the "vibrations" at 0K must be of the order of:

$$c_D^2 = \frac{L^3 \hbar \omega}{\beta EI} = \hbar \sqrt{\frac{2L^3}{\beta EI m_{eq}}} \quad (24)$$

with frequency given by eq. (13).

4. Non linear effects: the horizontal vibration of the tip and the stretching

Clamped-clamped NEMS presents a symmetric vibration, whereas for cantilever NEMS the oscillation is not symmetric, as a consequence of the large displacements of the tip, having also a horizontal component. Since:

$$ds^2 = dz^2 + dw^2 \quad (25)$$

and assuming for cantilever NEMS:

$$w(s) \approx \frac{s^2}{L^2} c \quad (26)$$

(note that this simple form can be used to compute the electrostatic and van der Waals energies but not the elastic energy, since it involves a second order derivative of w) it follows:

$$\left(1 - \frac{4c^2}{L^4} s^2\right) ds^2 = dz^2 \quad (27)$$

Integrating the square root of eq. (27) as:

$$\int_0^L \left(1 - \frac{2c^2}{L^4} s^2 - \frac{2c^4}{L^8} s^4\right) ds \cong \int_0^{L-\Delta} dz, \quad (28)$$

yields the estimation of the horizontal displacement Δ of the tip:

$$\Delta \cong \frac{2}{3} \frac{c^2}{L} \quad (29)$$

Thus, the vibrating position vector of the tip is described by (Δ, c) . Only for small displacements $\Delta \cong 0$. On the other hand, for clamped-clamped nanotube the energy due to stretching $\frac{N^2 L}{2EA}$ has to be added to the (linear and due to bending) contribute in eq.

(12). Accordingly, $E_{elast} \rightarrow E_{elast} \left(1 + \chi \frac{Ac^2}{I}\right)$ where χ is a parameter that can be derived assuming a mode shape for $w(s)$; a rough estimation is $\chi \approx 128/3003$ [13].

5. Free-energy of the NEMS

To quantify the approach proposed in the previous sections, it is sufficient to derive the expression of the free-energy of the NEMS. This step represents the aim of the present section. The elastic energy is given by eq. (12). Let us focus the attention on the cantilever geometry.

The free-energy of the NEMS has to be written as:

$$W(c) = E_{elast}(c) - E_{elec}(c) - E_{vdW}(c) \quad (30)$$

If the gaps are smaller than ~ 1 nm the Pauli's energy $E_P(c)$ (with a minus sign) has to be added in the right hand side of eq. (30).

For computing the electrostatic energy, we assume a uniform charge distribution. Charge concentration at the free-end of the cantilever nanotube, as well as tunneling current, field emission and quantum effects are neglected (some information can be

found in [14-19]). In addition, we reasonably assume that the nanotube's (external) radius R is much smaller than the distance r between nanotube and ground plane, i.e., $R/r \ll 1$. By this assumption eq. (1a) becomes:

$$\frac{dE_{elec}}{ds} \approx \frac{\pi\epsilon_0 V^2}{\ln\left(\frac{2r}{R}\right)} \quad (31)$$

Noting that $r = H - w$ (and $R/H \ll 1$) the electrostatic energy per unit length becomes:

$$\frac{dE_{elec}}{ds} = \frac{\pi\epsilon_0 V^2}{\ln\left(\frac{2H}{R}\right)} \left(1 + \frac{1}{\ln\left(\frac{2H}{R}\right)} \sum_{i=1}^{\infty} \frac{1}{i} \left(\frac{w}{H}\right)^i \right) \quad (32)$$

The total electrostatic energy stored in the nanotube, according to eqs. (26) and (32), can be expanded in series as:

$$E_{elec}(c) = \int_0^L \frac{dE_{elec}}{ds} ds = \frac{\pi\epsilon_0 V^2 L}{\ln\left(\frac{2H}{R}\right)} \left(1 + \frac{1}{\ln\left(\frac{2H}{R}\right)} \sum_{i=1}^{\infty} \frac{1}{i(2i+1)} \left(\frac{c}{H}\right)^i \right) \quad (33)$$

In contrast, according to our previous hypothesis, $R/r \ll 1$, eq. (1b) can be rewritten as:

$$\frac{dE_{vdW}}{ds} = \pi^2 C_6 n^2 d^2 N_w \langle R \rangle \sum_{r=r_{int}}^{r_{int} + (N_G - 1)d} r^{-4} \quad (34)$$

where N_w is the number of walls of the nanotube and $\langle R \rangle$ is the mean value of their radii.

Analogously, for the van der Waals forces:

$$\begin{aligned} \frac{dE_{vdW}}{ds} &= \pi^2 C_6 n^2 d^2 N_w \langle R \rangle \sum_{i=0}^{N_G - 1} (H + id)^{-4} \left(1 - \frac{w}{H + id} \right)^{-4} \\ &\approx \pi^2 C_6 n^2 d^2 N_w \langle R \rangle \sum_{i=0}^{N_G - 1} (H + id)^{-4} \sum_{j=0}^{\infty} \binom{-4}{j} \left(-\frac{w}{H + id} \right)^j \end{aligned} \quad (35)$$

By employing eqs. (26) and (35), the total van der Waals energy accumulated in the tube is:

$$E_{vdW}(c) = \int_0^L \frac{dE_{vdW}}{ds} ds = \pi^2 C_6 n^2 d^2 L N_w \langle R \rangle \sum_{i=0}^{N_G - 1} (H + id)^{-4} \left(1 + \frac{4}{3} \frac{c}{H + id} + \dots \right) \quad (36)$$

where the linear term in c represents the first corrective factor for accounting the van der Waals forces. Thus, the free-energy of eq. (30) is now quantified, and the amplitude and frequency of the oscillations, according to Section 3, can be evaluated. Note that, the free-energy of eq. (30) must be rewritten, according to our hypothesis of $W(c_S) = 0$, where $c_S : \left. \frac{dW(c)}{dc} \right|_{c=c_S} = 0$, before applying the relationships derived in Section 3. The same estimations for the electrostatic and the van der Waals energies are found for a half clamped-clamped nanotube of length $2L$ if we assume still valid for the symmetric deflection the form of eq. (26). Since such estimations are linear in L , in this assumption, they are still valid for a clamped-clamped nanotube of length L . Obviously, as for cantilever, more realistic forms (e.g., satisfying the congruence of the rotations) have to be considered, at least, in computing the elastic energy, as done in Section 4.

5.1 Pull-in voltage prediction

Thus the free-energy is now well-defined and we can apply eq. (17); accordingly, we find the pull-in voltage for:

$$V_{PI} = k\sqrt{1+k_{NL}} \frac{H}{L^2} \ln\left(\frac{2H}{R}\right) \sqrt{\frac{\beta EI}{\epsilon_0}} \quad (37)$$

where $k \approx 0.85$ and k_{NL} describes the non linear effects treated in Section 4 (for the linear case $k_{NL} \approx 0$); as a first approximation $k_{NL} \approx H^2/L^2$ for the cantilever whereas $k_{NL} \approx \frac{1}{100} \frac{AH^2}{I}$ for the clamped-clamped devices, showing the tremendous influence of the stretching ($\sqrt{I/A} \ll L, H$ is of the order of R). Here we have neglected the van der Waals forces, that have to be considered only for gaps (technologically still unrealistic) lower than ~ 10 nm. However, considering the first corrective term for accounting the van der Waals forces, we find the instability at V_{PI}^{vdW} , presenting a shift with respect to V_{PI} given by:

$$\Delta^{vdW} V_{PI} = V_{PI} - V_{PI}^{vdW} \approx 2nd \ln\left(\frac{2H}{R}\right) \sqrt{\frac{C_6 H N_w \langle R \rangle \sum_{i=0}^{N_G-1} (H+id)^{-5}}{\epsilon_0}} \quad (38)$$

6. Comparison with experimental and numerical results

Usually, free and thermal vibrations of nanotube based NEMS are studied around the relaxed configuration, due to the higher complexity in treating the effect of the electrical field and van der Waals forces in the dynamics of the system. Neglecting such effects, the classical approach to study the free (or thermal, by virtue of the Equipartition Theorem) vibrations of the beams holds. The proposed approach allows us to estimate the effect of the external fields as well as the “vibrations” at 0K of NEMS. Another important result is the prediction of the pull-in, corresponding to the on/off transition of the system, eq. (37), a key design parameter for the NEMS.

Some interesting experimental observations of free thermal vibrations for singly and doubly clamped nanotubes were reported respectively by Chopra and Zettl [3] and Babic et al. [20]. For the cantilever nanotube $E \approx 1.2\text{TPa}$, $L \approx 154\text{nm}$, $R = R_{ext} \approx 1.75\text{nm}$, $R_{int} \approx 1.1\text{nm}$ and, according to eq. (16), the amplitude of the thermal vibrations at 300K of the free-end is estimated to be of the order of $\sim 1.4\text{nm}$; the root mean square amplitude (obtained by dividing for $\sqrt{2}$) is consequently of the order of 1nm , close to the observed value of $\sim 0.8\text{nm}$. The frequency ($P^{-1} = \omega/(2\pi)$), according to eq. (13), is estimated to be of the order of $\sim 0.4\text{GHz}$. Finally, the vibrations at 0K, according to eq. (24), are estimated to have amplitude of the order of $\sim 0.05\text{\AA}$.

For the clamped-clamped nanotube $E \approx 1\text{TPa}$, $L \approx 6.25\mu\text{m}$, $R = R_{ext} \approx 1\text{nm}$, $R_{int} \approx 0.665\text{nm}$ and, according to eq. (16), the amplitude of the thermal vibrations at 300K of the free-end is estimated to be of the order of $\sim 0.13\mu\text{m}$ (rms), close to the observed value of $\sim 0.08\mu\text{m}$. The frequency, according to eq. (13), is estimated to be of the order of $\sim 0.7\text{MHz}$. Finally, the vibrations at 0K, according to eq. (24), should have amplitude of the order of $\sim 0.2\text{\AA}$ (note that these comparisons simply assume the reported rough estimations for the parameters α , β and $\rho_m = 2260\text{Kg/m}^3$; better estimations could be easily obtained considering more realistic forms for $w_S(s)$).

Since no extensive investigations on dynamics of nanotubes under external fields are present in literature, an additional possibility to check the analysis can be achieved by comparing the prediction of the instability given by eq. (37) with a linear numerical analysis [10], for which $E = 1.2\text{TPa}$, $R_{int} = 0\text{nm}$, $L = 50\text{nm}$, $R = 1\text{nm}$, $H = 4\text{nm}$. The comparison is reported in Figures 2 and 3 by varying the length and the gap of the NEMS. We conclude that theory and numerical results agree satisfactorily.

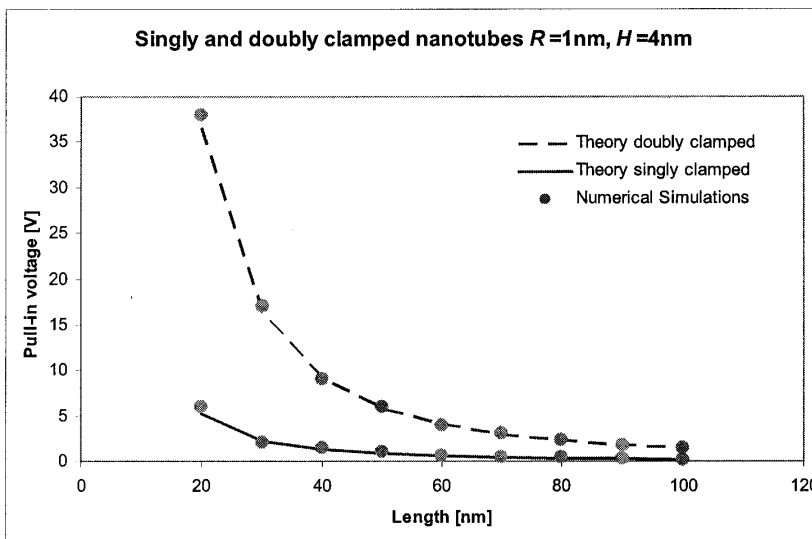


Figure 2. Comparison between theory and numerical simulations for the pull-in voltage as a function of the horizontal size (L) of the device.

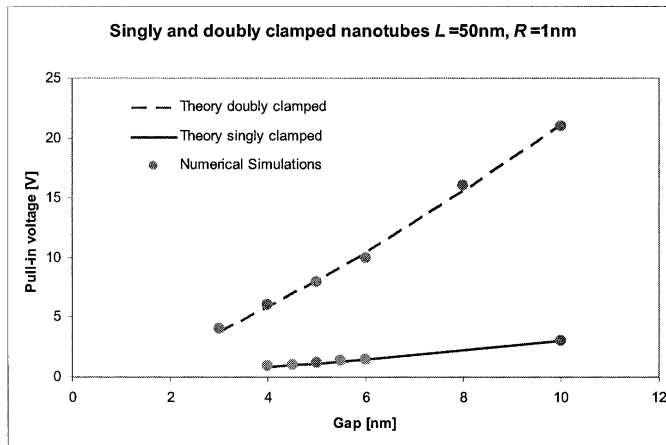


Figure 3. Comparison between theory and numerical simulations for the pull-in voltage as a function of the vertical size (H) of the device.

7. Conclusions

In this paper the non-linear dynamics of nanotube based NEMS has been investigated. The vibrations of NEMS have been studied considering large displacements, the effect of the electrical field and of the van der Waals forces. The NEMS free-, thermal- and at 0K oscillations have been consequently analyzed. A comparison with experimental observations on thermal vibrations for both singly and doubly clamped nanotubes has been shown. The estimations of the amplitude for the corresponding vibrations at 0K have been also deduced. The free-energy based approach has been verified by setting to zero the frequency of the oscillations, corresponding to the collapse of the device at the so-called pull-in voltage, and by comparing the results with numerical simulations. The pull-in voltages calculated show a relevant agreement with the numerical computed values.

The influence of the non linear effects on the pull-in voltage has been also predicted. A comparison with the numerical solution of the non linear equation (4) will be presented in the future. We conclude that the proposed approach could be useful in the design of NEMS.

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