Nanotube MEMS: Modeling extreme nanoscale devices

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ABSTRACT

The physics of operation of nanotube NEMS devices is reviewed. Special attention is paid to non-classical effects, rarely described in MEMS analysis, such as van der Waals/Casimir interactions, quantum effects in electrostatics, atomistic parameterization of elasticity. As an example of a breakdown of a classical MEMS theory, the NEMS scaling limitation is derived in a lump model taking into account van der Waals/Casimir attraction.

Keywords: nanotube devices, MEMS/NEMS, theoretical, van der Waals/Casimir forces

1. INTRODUCTION: NEMS VERSUS MEMS

Far from reaching its limits, MEMS technology proved itself in various applications, ranging from car acceleration and pressure sensors to space telescope shutters. Nowadays MEMS devices approach nanometer scale, promising even larger versatility, including hybrid THz-electronics, low-power memories and sensors with record sensitivity. Common name for nanoscale MEMS is NEMS, although no clear distinction of the latter versus the former is found in literature. For the purpose of this paper we use the following definition of NEMS: an electromechanical device which has such a small size scale (typically of the order of nanometers) that non-classical effects may take place and furthermore become important for the device operation. Among those effects we name van der Waals/Casimir (vdW/C) forces, quantum effects in the charge distribution (including but not limited to the quantum capacitance, Coulomb blockade and charge tunneling), breakdown of the bulk elasticity theory. This list cannot be complete because the NEMS science is still developing and new discoveries are foreseen that could open unexplored routes to new evolutionary and revolutionary device technologies.

While NEMS devices have large potential, their engineering enters a new territory, full of surprises and paradoxes. This paper is devoted to the new physics of device operation that involves understanding of few fundamental concepts, rarely illuminated in MEMS literature in the past.1 (We note that the problems of nanofabrication and controlling the matter at the nanoscale are equally important but fall beyond the scope of the paper).

Quantum (and surface microscopic) effects may appear in NEMS due to the size of device (or at least operational part of it) is comparable with a size of atoms/unit cells of the materials used to fabricate it. In addition, device size may become smaller than some characteristic length associated with the electronic or mechanical properties of the material, for example, a Deby screening length, or a thickness of the shell for layered materials. In these cases the classical textbook description may become incomplete and few of such examples will be reviewed below.

At the same time, classical models, like the beam and shell mechanics, continue work surprisingly well beyond projected atomic-scale limits, as we will demonstrate for nanotube NEMS. We will show that even in the case of a quantum charge distribution influencing the coupling between the NEMS channel and the ground plate one can introduce an effective (quantum) capacitance which differs though from the classical one. Thus appropriately modified “classical” models may serve for understanding NEMS operation.

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2. OPERATION OF NANOELECTROMECHANICAL SWITCHES

Various (carbon, nitride, and chalcogenide) nanotubes are the shell structures of cylindrical shape with very large aspect ratio, showing unusual mechanical and electronic properties, stability, and functionality. The lattice structure of single-wall carbon nanotubes (SWNT) is the same as in graphene (monolayer of graphite): a hexagonal chicken-wire lattice which consists of only carbon atoms. A translational symmetry along the tube axis is augmented with axial (or spiral) symmetry along the NT circumference.

![Figure 1. Bandstructure of an armchair metallic SWNT [10,10] (Right) and a zigzag semiconducting SWNT [17,0] (Left) within first Brillouin zone, $k$ is electron axial momentum, $b$ is the carbon-carbon bond length. Energy is in units of $\gamma \approx 2.7$ eV, tight-binding hopping integral. Inset: Geometric structure of the same SWNTs.](image)

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Multiple examples from the physics of carbon nanotube (NT) NEMS, including both existing and theoretically proposed devices, will be given below. Natural size of a single NT is small enough so the quantum effects are easy to observe. For example, a finite value of the electronic density of states results in breaking the classical electrostatics and brings a NT quantum capacitance term. The transverse size of the shell of the NT may be as small as one monolayer of graphene thus a special attention will be paid to the NT elasticity theory. We will review novel effects which differentiate NT-NEMS from their classical MEMS counterpart. Van der Waals/Casimir forces will be discussed in the context of a fundamental physical limit for scaling down NEMS-actuators.

Layered carbon materials, such as fullerenes, nanotubes and graphene, have two types of valence electrons: pi and sigma electrons. The sigma electrons are localized, make strong chemical bonds and thus contribute to the excellent mechanical properties. Pi-electrons are mobile and highly polarizable and define electrical, optical and electromechanical properties. In NTs it is the pi-electrons’ 2D structure of graphene, which becomes a series of the one-dimensional (1D) subbands due to the orbital quantization along the NT circumference, and determines the electronic charge (Figure 1).

![Figure 2. Force balance for a OFF state of a nanotube electromechanical switch (a single arm horizontal cantilever). Arrows show applied forces: electrostatic, van der Waals/Casimir, and elastic forces. (Upper inset) Nanotube nanotweezers device. (Lower inset) Comparison of a single NT NEMS and a parallel array NT NEMS.](image)

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Three main geometries employed in NT-NEMS fabrication are a suspended multiple- or single-NT bridge, tweezers and a single arm NT cantilever, horizontal or vertical (We note that at the nanoscale the gravity is of no importance because of too small masses of the bodies, therefore, there is no conceptual difference between the horizontal and vertical placement). Experimental realizations of various horizontal and vertical switches, NT DRAMs and nano-relay have been reported. Shown in Figure 2 is the nanoelectromechanical operation of a simplest horizontal single-arm cantilever switch. The switch consists of a moveable structure, which can be a single wall or a multiwall carbon nanotube, and a fixed ground plate, which was modeled, for example, by a graphite bulk in Ref. When a potential is applied between the moveable structure and the ground plate, electrostatic charges are induced on both the movable structure and the ground plate. The electrostatic charges give rise to electrostatic forces, which deflect the movable NT.

This classical picture implicitly presumes that an arbitrary charge can be added to (subtracted from) the NT which does not take into account a quantum nature of an electron.

In addition to electrostatic forces, depending on the gap between the moveable tube and the ground plate, the van der Waals/Casimir forces also act on the NT and deflect it. For a normal case of attractive vdW/C force, the directions of the electrostatic and vdW/C forces are the same and are shown in Figure 2.

Counteracting these forces are elastic forces, which try to restore the NT to its original straight position. In MEMS modeling a classical finite element (FE) would be applied to compute this response. At nanoscale, it is not though obvious how the FE modeling should be parameterized, bulk elastic parameters may not be accurate and should be replaced for NEMS.

For a given applied voltage, an equilibrium position of the tube is defined by the balance of the elastic, electrostatic, and van der Waals forces. As the NT deflects, all forces are subject to change, and a self-consistent analysis is necessary to compute the equilibrium position of the NT as found from the zero force condition or, alternatively, as the minimum of the total energy. Such a solution is unique for low potential difference between the NT and the ground plate. When it exceeds a certain critical value, the solution becomes unstable (bi-valued) and the NEMS collapses onto the ground plate. Such critical potential is called the pull-in voltage. When the pull-in voltage (or higher) is applied, the NT comes in contact with the ground plate, and if it is conductive the device is in the ON state. When the potential is released, and if the elastic force is strong enough to overcome the vdW/C force at the zero separation, the NEMS moves in the original OFF state (Figure 2). The significant difference with the MEMS device is in the vdW/C forces, which can result in the sticking of NEMS device in the ON position. This can limit the range of operability of NEMS. If the gap between the cantilever tube and the ground plate is too small, even without an applied voltage, the NT can collapse onto the ground plate because of the vdW/C forces.

3. NANOTUBE MECHANICS: ATOMISTIC VS. CONTINUUM MODELING

Mechanical properties of NTs are subject of intensive experimental and theoretical studies. Multiple numerical solution techniques have been developed recently to model the NT mechanics in NEMS. In this paper we will focus on conceptual aspects of NEMS modeling rather than provide a detailed review of the field. Elastic and structural properties of NT systems have been studied both theoretically and experimentally over the last decade. Mechanical behavior of a small structure differs from that of a bulk material. New phenomena such as super-low friction, super-high stiffness, and high cohesion at small distances have been encountered.

The mechanical behavior of nanotubes can be modeled either by simple continuum approaches or by more complex atomistic approaches based, for example, on molecular dynamics simulations. Atomistic approaches have the advantage of capturing the mechanical behavior accurately; however, they require large computational resources. Continuum theories, when properly parameterized and calibrated, can be significantly faster and for device simulation much more efficient. A simple continuum approach to model nanoelectromechanical switches is based on the beam theory. The beam equation is given by:

$$\mu A \frac{\partial^2 x}{\partial t^2} + EI \frac{\partial^4 x}{\partial l^4} = F$$  \hspace{1cm} (1)
where \( x(l) \) is the gap between the conductor and the ground plate, \( l \) is the position along the NT, \( A \) is the cross-sectional area, \( \mu \) is the 3D mass density, \( F \) is the normal component of the force per unit length, \( E \) is the effective Young’s modulus (to be defined later), and \( I \) is the moment of inertia and, for a cylinder, can be estimated as:

\[
I = \frac{\pi}{4} (R_{\text{ext}}^4 - R_{\text{int}}^4)
\]  

(2)

where \( R_{\text{int}} \) is the interior radius and \( R_{\text{ext}} \) is the exterior radius of the NT which is well defined for the case of multiwall NT; for single-wall NT (SWNT) an atomistic dynamic modeling is required to evaluate \( I \) accurately.

What are the limitations of the beam theory? The NT buckling (forming the kinks at the clipped edge) at the loads exceeding the Euler critical load is expected.\(^{28}\) This however is a rare case for well-tempered NEMS device operation. Besides, more advanced mechanical theory can be applied to solve this difficulty.\(^{24,28,29}\) More importantly, the mechanics parameters for the beam theory have to be obtained by atomistic modeling rather that inherited from the macroscopic approach.

For example, the Young’s modulus of the SWNT cannot be defined unambiguously because this is a bulk macroscopic quantity which requires an averaging of the local mechanical properties of the material over a small but though macroscopic volume, containing many atoms.\(^{30}\) This quantity is often ill-defined in nanosystems. For example, definition of \( E \) for a single monolayer of graphene or a NT requires to define a thickness of the monolayer (cf. Ref.\(^{24}\) and references therein). The solution is in computing the mechanical materials constants that are independent of such non-physical quantities. For example, the cross-sectional area of a SWNT \( A \) in Eq. (1) cannot be defined properly, however, the product \( \mu A \) is well-defined, it is the mass-per-unit-length of the NT. Similarly the product \( EI \) has a direct physical meaning of a flexural rigidity of the NT and was computed numerically in Ref.\(^{31}\) by applying bending load to the NT within Molecular Dynamics (MD) simulation and fitting the deflection curve with the elastic beam response. Paper\(^{16}\) further extends this result for a tensile load allowing to obtain the product \( AE \) (we stress that still one cannot define these two quantities separately without making an ambiguous definition for the NT wall thickness). Simple parameterization has been proposed for flexural and also tensile rigidity of SWNTs in Ref.\(^{32}\) \( EI/d^3 \approx 0.14 \) TPa.nm and \( AE/d \approx 1.09 \) TPa.nm, where explicit dependence on the NT diameter \( d \) has been subtracted (notice that the scaling is the same as for an elastic shell structure with the cross-sectional area \( \propto 2\pi d \) not \( \pi d^2/4 \) as a thick cylinder).

4. VAN DER WAALS/CASIMIR INTERACTIONS

Main distinct feature of the NEMS operation is in appearance of fluctuation (vdW/C) forces and a dominant role of these forces in some range. The vdW/C interactions have quantum-mechanical origin and therefore largely neglected for macroscopic systems. Furthermore, theoretical description of the vdW/C interactions is complicated, metal and insulating, bulk and atomic systems are treated differently, no simple and unified theory has been developed so far.\(^{33}\)

We have pioneered modeling of vdW/C forces for NT-NEMS. The first paper Ref.\(^{15}\) proposed a simple approach to include it through, so called, Lennard-Jones 6-12 potential. This is an empirical interatomic potential\(^{34}\) which was shown to describe interactions between individual atoms and, when integrated over all atomic positions, the interactions between the solids. In Ref.\(^{35}\) a method was developed to split the part which depends on the materials property of the carbon atoms (for graphitic systems) and the geometry of interacting objects, the shell geometry for NTs. In Ref.\(^{16}\) the method was combined with the MD mechanics and classical electrostatics to obtain an atomistic response of the NT-NEMS. Main drawback of the Lennard-Jones approach, however, is in incapability to reflect the many-body nature of the vdW/C forces which are non-additive themselves, that is the interaction is not a pairwise sum of an atom-to-atom two-center potentials.\(^{33,36}\) Most of NEMS modeling up today neglects this issue, though.

Many-body corrections to vdW/C interactions from non-additive surface plasmon-polariton modes between NT and a metal substrate were calculated and applied in the continuum modeling of NTs in Ref.\(^{37}\) A simple yet very effective model has been developed to estimate a major portion of the total vdW/C energy, which is due to the plasmon-polariton modes having a large oscillator strength. Quantum electrodynamics approach\(^{33}\) allows to relate the vdW/C potential to the absorption coefficient of the medium which is, in turn, dominated by the modes of the largest oscillator strength.
Two interesting phenomena were discovered in the course of this study. We have modeled several systems (shown in Figure 3): a double-wall nanotube, a nanotube on the metal surface, and a pair of SWNTs. A significant difference of the distance dependence of the vdW/C energy, as compared to the classical 6-12 potential, was found. This has been more recently confirmed in an independent study. 

Pairwise summation approach gives the energy scaling as \( W \propto x^{-5} \) for a couple of purely 1D systems (two interacting wires) and \( W \propto x^{-4} \) for a wire over a plate (1D-to-2D). We have shown for the first time that for the NT 1D plasmons the vdW/C energy scales as \( x^{-4.5} \) for the interaction between a NT and a metal substrate and it is \( x^{-4.5} \) for the attraction between two NTs.

![Figure 3](image-url) Distance scaling of a plasmonic component of the van der Waals/Casimir energy (log-log plot). (Insets) Geometry of two of the studied NT systems: (lower) an interaction between SWNT and a metal ground plate; (upper) an interaction between two SWNTs.

### 5. ELECTROSTATICS: CLASSICAL AND QUANTUM TERMS

The three-dimensional character of the electromagnetic field and one-dimensional charge density distribution of a SWNT result in a weak screening of the external field, yet non-negligible. To compute the electrostatics domain of the energy of a NEMS we need a relation between the induced charge density in the NEMS channel and the external applied potential. It must be calculated quantum mechanically, in general, by computing the local Density of States (DoS). Though for not too strong electric fields that do not induce large dipole across the SWNT and do not modify the original bandstructure of the SWNT, that is, do not change the dispersion law for valence electrons, an effective capacitance theory can be developed.

Raw NT material, as synthesized, contains both metallic and semiconducting NTs (Figure 1). The dispersion relation for low energy electron in a semiconducting SWNT is

\[
\varepsilon(k) = \sqrt{\left( \frac{\hbar v_F^2}{2} k^2 \right) + \Delta^2}
\]  

where \( k \) is the linear axial momentum of the valence electron counted from the top (bottom) of the valence (conduction) band, \( \hbar \) is the Planck constant, \( v_F \) is the Fermi velocity (the electrons in graphene and SWNT are described with an effective Dirac, pseudo-relativistic, Hamiltonian; \( v_F \) plays the role of the "speed of light" in graphitic systems), \( 2\Delta \) is the semiconductor band gap. The local DoS (at low \( \varepsilon \)) is given then by the expression:

\[
g(\varepsilon) = (\partial \varepsilon / \partial k)^{-1} = \frac{1}{\hbar v_F \sqrt{\varepsilon^2 - \Delta^2}} = g_0 \frac{\varepsilon}{\sqrt{\varepsilon^2 - \Delta^2}}.
\]  

For NEMS device, if we consider only the middle part of the channel, far away from the screening metal contacts, which stipulates that the DoS is unperturbed one as for the pristine SWNT in the vacuum, we can compute the charge density, \( \rho \), as a function of the electrochemical potential \( \zeta \), taking into account the temperature effects in the lowest order:

\[
\rho(\zeta) = e \int f(\zeta) g(E) dE = \frac{e}{\hbar v_F} \int \frac{E f(\zeta)}{\sqrt{E^2 - \Delta^2}} dE = -\frac{C_Q}{e} \sqrt{\zeta^2 - \Delta^2} + O\left( \frac{T^2}{\Delta^2} \right)
\]
where \( f(\zeta) = 1/(1 + \exp[(E - \zeta)/(kT)]) \) is Fermi-Dirac distribution function. We derived the SWNT quantum capacitance \( C_Q = e^2/\hbar v_F \) as a coefficient, related to the local DoS.\cite{17,39,41} Next, one has to determine the value of \( \zeta \) as a function of applied external potential, \( \varphi_{xt} \). Often, a rough approximation is used: \( \zeta \rightarrow -e\varphi_{xt} \) which holds only for some extreme limiting cases, as we demonstrate next, but it is not a valid approximation for a NEMS in general. More precisely, \( \zeta + e(\varphi_{xt} + \varphi_{ind}) = 0 \) where two terms in brackets constitute the total acting potential, \( \varphi_{act} \).

Great simplification is achieved in case of the metallic nanotube. If device is operating at a low voltage when \( \zeta \) is within the lowest metallic subband where the dispersion law is linear: \( \varepsilon = \hbar v_F k \), then the density of states is constant, \( g_o \) (see Figure 4) and the induced charge density reads as:

$$
\rho(z) = -e^2 g_o \varphi_{act}(z) = -C_Q \varphi_{act}
$$

(6)

Although, Eq.(6) gives an exact charge density only in the case of the Fermi level crossing the first (lowest) subband of the metallic NT, we note that the other singularities of the one-dimensional DoS are integrable. It means that for practical applications the approximate linear dependence of the charge density on the acting potential holds across the whole voltage (local electrochemical potential) range, with the possible exception in a small region at the subband edge, though the coefficient is not simply \( C_Q \) but varies with \( \varphi_{xt} \).

The induced component of the total acting potential is readily derived from the charge density via the Poisson integral:

$$
\varphi_{ind}(r) = 4\pi \int G(r, r') \rho(r') \, dr'
$$

(7)

where \( G \) is the Green’s function of the Coulomb interaction (the formal solution of the Poisson equation for the given device geometry). Standard methods can be used for solving this equation.\cite{39,41,42}

The Green’s function of a 1D system is known to have a logarithmic singularity at large distance unless some external screening is considered. In case of a NEMS device, this screening is due to the closest gates/contacts. An equation, giving the NT charge density implicitly, reads as (compare Eqs.(6,7) and a definition \( \varphi_{act} = \varphi_{xt} + \varphi_{ind} \)):

$$
-\frac{\rho(r)}{C_Q} - 4\pi \int G(r, r') \rho(r') \, dr' = \varphi_{xt}(r).
$$

(8)

The equation can be inverted analytically only in a simple case. The numerical study has been performed in Ref.\cite{42} An interesting result is that the NT NEMS channel may be divided in three parts: the side regions and a central region. The side parts are the regions near the contact (or near the free end of a cantilever NT) of a length about several \( h \) long, where \( h \) is the distance to the metal plate. Aspect ratio of the state-of-the-art NT NEMS devices is very large, which means that the axial size of the NT, \( L \), is much longer than the \( h \). Then,

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**Figure 4.** Schematic DoS of a metallic SWNT. First subband contributes to a constant DoS at the \( E = 0 \). An injected/induced charge is proportional to the shaded area and is a linear function of the electrochemical potential, \( \zeta \), when \( \zeta \) is lower than the second subband edge.

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the central region of the nanotube covers most of the device length. In the central part the electrostatics is elementary which allows an elegant analytical solution:

$$\varphi_{ind}(r) \approx 4\pi \rho(r) \int G(r,r')dr' = \rho(r) C_g^{-1}$$

(9)

here the charge density $\rho$ adiabatically follows the external potential $\varphi_{xt}$. Thus the integral depends on the system geometry only (and is independent of $\rho$ and $\varphi_{xt}$). We have shown that this integral equals the classical electrostatic capacitance (per unit length) of the NEMS channel.

Figure 5. Schematic geometry of two single-wall NT devices studied in the section: (A) cantilever NEMS, and (B) bridge NEMS. The nanotube is substantially longer and more narrow (not shown to scale). Induced charge density distributions for these device are plotted in the next figure.

Then, the self-consistent equation for the charge density is:

$$\rho \approx -\frac{\varphi_{xt}}{C_g^{-1} + C_Q^{-1}} \approx \rho_{cl} \left(1 - \frac{C_g}{C_Q}\right)$$

(10)

where $\rho_{cl} = -C_g \varphi_{xt}$ is the classical charge density in a thin metallic cylinder in the same device geometry. For the straight SWNT in vacuum: $C_g^{-1} = 2 \log \left(\frac{2h}{R}\right) \gg 2 \log 2 \sim 1.4$, where $R$ is the NT radius, and the quantum term, $C_Q^{-1} = \hbar v_F/e^2 \sim 0.3$, is much smaller, which allows one to expand the total capacitance in series in $C_g/C_Q \ll 1$. In the limit of infinite DoS ($g_o \to \infty$ or $C_Q \to \infty$) the quantum term disappears and we retain the classical relation for a bulk metal.

The equation for the equilibrium charge density is valid for a distorted nanotube as well as for an ideal straight nanotube, although no simple expression for the geometric capacitance can be written. In the case of slightly bent SWNT, one can use $C_g^{-1}(h(z))$, capacitance of the bent metallic cylinder, in Eq.(10) instead of the logarithmic capacitance which is valid only for a straight NT. The function $h(z)$ gives the NEMS deflection from the equilibrium shape which determines the local capacitance coupling to the ground plate. (We neglect here that the mechanical perturbation can result, in principle, in an appreciable change in the DoS/electronic properties.5 Though in case of a weak strain the quantum capacitance of the distorted SWNT indeed remains the same). Then the total capacitance depends on the NT shape via the geometrical term only:

$$C(z) \approx \frac{1}{C_g^{-1}(h(z)) + C_Q^{-1}} \approx C_g(z) \left(1 - \frac{C_g(z)}{C_Q}\right).$$

(11)

This analytical form of self-consistent solution for the device electrostatics is very useful for calculating electrostatic forces in various NEMS devices.

Recently NT DRAM elements have been fabricated with a gate in a form of a semi-enclosing sheath around a multiwall NT (Figure6). We note that a geometrical capacitance has a weak (logarithmic) dependence on the actual geometry of the device, being mostly determined by its size scale. Thus most of our analysis is directly applicable for these memory devices.

Edge effects were also studied to reveal the dependence of the total capacitance on the geometry of the finite length NT (once again we assume that the DoS does not change for the finite length SWNT which may
be not always the case). Charge distribution of the classical thin wire becomes very nonuniform at the ends of the cylinder of the finite length, also known as a fringe field effect or a field enhancement. As a result, a field emission may begin at the free NT end or even at the point of closest proximity to the metal plate, depending on the NEMS geometry and applied potential (in Ref. 44, we provide Fowler–Nordheim parameters for SWNT to estimate the field-emission current at a given value of the field). Taking as a rough estimate that a critical field \( \sim 5 - 10 \text{ V/nm} \) is required, we can conclude that for a 1 nm wide SWNT this may happen at \( \sim 5 - 10 \text{ V} \) applied between the NT and the plate. This would restrict the operational range of NT NEMS.

We derived the self-consistent solution for the charge density in a metallic SWNT. Similar equation can be derived for a semiconductor SWNT:

\[
\rho(\varphi_{xt}) = -eC_Q \varphi_{xt} B(\varphi_{xt})
\]

where the non-metallicity factor \( B(\varphi_{xt}) \) is a complicated function of the ratio \( e\varphi_{xt}/\Delta \) and also \( C_g/C_Q \). It replaces the factor \( C_g/(C_Q + C_g) \) in the metallic SWNT and corrects for the difference in charge coupling in the semiconductor SWNT and in an ideal bulk metal.

NEMS devices with a single NT as a channel are attractive due to their ultimately small size and expected low power consumption and fast operation, but more practical, though larger in size, multiple NT devices have been also considered. Ref. 45 discusses possible bundling instability in a theoretical parallel microbeam array. Such structures can be fabricated nowadays thanks to a breakthrough synthetic technique discovered recently. 47

Changing the SWNT type (from metallic into semiconductor) one has to change the materials parameter \( C_Q \) which depends on the DoS. In a similar way, changing NEMS geometry from a single NT bridge to a parallel array of NTs (Figure 6) one has to replace the geometrical capacitance term, \( C_g \), with an effective capacitance of an (infinite) circuit shown as inset in the Figure. Analytical formula for an effective capacitance of a parallel NT array has been derived in Ref. 48

\[
C^{-1}_{\text{array}} = 2 \log \left( \frac{\Lambda_o \sinh \pi 2h/\Lambda_o}{R} \right)
\]

where \( \Lambda_o \) is an average distance between NTs in the array.

**Figure 6.** (Right) A scheme of a NT memory device. The sheath gate replaces the ground plate for this vertical NEMS switches. (Left) The parallel array of NTs for a bridge NEMS. The effective capacitance circuit of the array-NEMS is shown on top.

Quantum effects may become important for the short NEMS devices when the space quantization along the channel is non-negligible. Figure 7 shows the NT induced-charge density computed in Ref. 49 by solving joint Shroedinger and Poisson equations for the valence electrons of a metallic armchair \([10,10]\) SWNT, 50 nm long, bridging the electrodes, or, 50 nm long, suspended from one side-electrode, at the distance 5 nm from the ground plate. These two NEMS devices have been modeled in one subband approximation (in full neglecting the intersubband or sigma–pi mixing, which has been estimated and was of minor importance for this problem).
The continuous line is the result of the statistical approximation. The quantum mechanical density is shown as an oscillating curve. It coincides with the analytical solution except for the quantum beating at the NT ends. Dashed line represents an analytical approximation, as in Eq.(10).

One can draw a conclusion that the quantum mechanical modeling can often be in qualitative if not in quantitative agreement with properly parameterized simpler semi-classical models.

Figure 7. Self-consistent charge density of a [10,10] armchair NT at 5 V voltage applied between side and back-gate contacts. The distance between the NT center and the back gate is 5 nm, and the NT radius is 0.6 nm and NT length is 50 nm (for the cantilever NEMS, left) and 40 nm (for the bridged NEMS, right). The solid oscillating (red) curve is a result of the quantum mechanical calculation. The solid (blue) line is a solution of joint Poisson and Boltzmann equations. The dashed (green) line is by the analytical approximation.

### 6. ANALYTICAL CONSIDERATION FOR THE PULL-IN

We finish this chapter with an analytical model that can be used for a quick estimation of pull-in voltages of the NT system within continuum modeling. Assuming that the elastic energy of the NEMS device is given by

\[ T = \frac{k}{2}(h - x)^2 \]  

where \( x \) is a lump coordinate to represent a NEMS deflection from the equilibrium. Assume that the external (electrostatic) force is the gradient of the energy component given by

\[ V = \frac{C}{2}\varphi^2 \]  

where \( C \) is the effective capacitance, including quantum terms. The electrostatic potential can be determined through the NEMS applied voltage \( V \) for given device geometry, as explained above. Then, we can calculate elastic and electrostatic forces. Next we include the van der Waals/Casimir energy term:

\[ W \simeq \varepsilon \frac{1}{x^\alpha} \]  

here we parameterize a general power law for vdW/C interaction via a characteristic energy, \( \varepsilon \), and the decay exponent, \( \alpha \), which may be determined by quantum electrodynamics (or by other methods).

Using this simple lump model with one variable, \( x \), and one input parameter, \( V \), we can write analytically the pull-in voltage, \( V_o \), and pull-in gap, \( x_o \), as functions of the NEMS effective stiffness, \( k \), the effective NEMS
capacitance, $C$, and van der Waals energy, $W$:

$$x_o = h A_1 \frac{1}{2} \left( 1 + \sqrt{1 + A_2 \frac{W(x_o)}{kh^2}} \right)$$

$$V_o = B_1 \frac{\sqrt{2kh^2}}{C(x_o)} \sqrt{\frac{x_o}{h A_1} - B_2 \frac{W(x_o)}{kh^2}}$$

where four constants $A_1$, $B_1$, $A_2$, and $B_2$ are derivatives describing the specific dependence of $C(x)$ and $W(x)$. In case of a planar switch and the classical Lennard-Jones potential, these constants are $2/3$, $\sqrt{2}/3$, 36, and 36, respectively. Neglecting the vdW/C term we obtain a classical result: $x_o = 2h/3$ and $V_o \propto h^{3/2}$.

This simple analysis allows already to explain the role of vdW/C interactions. As a result of the vdW/C attraction to the gate, the NEMS device cannot operate at very small gaps, $h$. The critical gap, $h_c$, (at which $x_o = h$) is about 2 nm for the switch with the following parameters $k \sim 1W/nm^2$, and $C \sim 2\sqrt{k}/(3V/nm)$. Figure 8 shows the self-consistent solution for the pull-in gap plotted vs. $h$, that is vs. the NEMS scale, because the gap is the smaller, the smaller is the whole device.

Figure 8. Operational range of the NEMS. The pull-in gap, $x_o$, is plotted as a function of the initial device gap (NEMS size), $h$. Solid (red) curve represents the self-consistent analytical result. Dashed line shows the classical dependence in neglecting the van der Waals correction: $x_o = 2h/3$. Dotted arrow shows the critical device size, $h_c$. (Lower inset) Unitless pull-in gap (in parts of the NEMS size), $x_o/h$. (Upper inset) The pull-in voltage, $V_o$, vs. NEMS size. Thin (green) line shows the classical result $V_o \sim h^{2/3}$. Shaded area is not accessible due to possible field emission from the NT.

7. CONCLUSIONS

Development of fast and precise approaches for three-dimensional device modeling of NT systems becomes clearly important given recent successes in creating prototypes for NT NEMS. The physics of carbon NT devices is rather distinct from the physics of standard MEMS. Various quantum and atomistic effects were shown to influence device operation. Certainly some NEMS effects have not been covered in this paper, for example, capillary fluctuation forces responsible for stiction, Coulomb blockade effect that can result in discretized pull-in behavior, various dissipation channels, challenges of high-frequency operation of NEMS switch, and many others.

Development of device modeling tools for NTs can be very complicated because of the breakdown of continuum theories. Molecular mechanics (MM) and molecular dynamics (MD) can be used reliably when continuum elastic
theories break down. Quantum mechanical Schrödinger equation has to be solved together with the Poisson
equation to obtain the self-consistent electrostatics. However, atomistic approach can be very computer time-
consuming. A good compromise is to develop a multiscale approach where continuum theories are combined
with atomistic approaches. Multiscale methods can be accurate and more efficient compared with atomistic
approaches.

We have reviewed in this paper atomistic parameterization schemes for NT-NEMS elasticity, electrostatics
and vdW/C interactions. The highest level in the multiscale hierarchy is represented by the quantum mechanical
theory for the NT response function, which is the atomistic analog of the bulk dielectric function. It contains the
complete information for the electronic structure and charge distribution and gives the means for calculating the
screened Coulomb and the van der Waals/Casimir forces. The main difficulty here is the requirement to solve the
problem for device structures. The electronic structure and the response function change during device operation,
and this requires a self-consistent treatment. At the intermediate level, classical molecular dynamics provides
a detailed knowledge for geometry and elastic parameters of the system. This is a prerequisite for calculating
the mechanical response of the system. It also supplies proper boundary conditions for electrostatic calculations
through the actual device geometry. At the lowest level of the simulation hierarchy continuum theories must
and can be applied. The parameters of the continuum models will, of course, need to be derived from the higher
level simulations.

ACKNOWLEDGMENTS

Author is greatly indebted to Professor Karl Hess and Professor Narayana Aluru for discussions on the topics
of the study. Author acknowledges partial support by DoD-ARL grant W911NF-07-2-0064 under Lehigh-Army
Research Laboratory Cooperative Agreement, National Science Foundation (CMS-0609050, NIRT), and the
Donors of the American Chemical Society Petroleum Research Fund (ACS PRF 46870-G10).

REFERENCES

1. Batra, R. C., Porfiri, M., Spinello, D., Review of modeling electrostatically actuated microelectromechanical
2. M. S. Dresselhaus, G. Dresselhaus, and Ph. Avouris, (Eds.), Carbon nanotubes: synthesis, structure, prop-
erties and applications, (Springer, 2001); M. Meyyapan, (Ed.), Carbon nanotubes: science and applications,
3. Dujardin, E., Derycke, V., Goffman, M. F., Lefevre, R., Bourgoin, J. P., Self-assembled switches based on
6. R. Lefevre, M. F. Goffman, V. Derycke, C. Miko, L. Forro, J. P. Bourgoin, and P. Hesto, ”Scaling Law in
10. J. E. Jang, S. N. Cha, Y. Choi, G. A. J. Amaratunga, D. J. Kang, D. G. Hasko, J. E. Jung, and J. M. Kim,
11. J. E. Jang, S. N. Cha, Y. Choi, T. P. Butler, D. J. Kang, D. G. Hasko, J. E. Jung, J. M. Kim, and G.
A. J. Amaratunga, "Nanoelectromechanical DRAM for ultra-large-scale integration (ULSI),” presented at
46. S.V. Rotkin, unpublished.