Designing a Double-Pole Nanoscale Relay Based on a Carbon Nanotube: A Theoretical Study

Weihua Mu (牟维华),^{1,2,*} Zhong-can Ou-Yang (欧阳钟灿),³ and Mildred S. Dresselhaus^{4,†}

¹School of Ophthalmology and Optometry, Eye Hospital, School of Biomedical Engineering, Wenzhou Medical University, Wenzhou 325027, China

²Wenzhou Institute of Biomaterials and Engineering, CNITECH, CAS, Wenzhou 325001, China

³Key Laboratory of Theoretical Physics, Institute of Theoretical Physics; Kavli Institute for Theoretical

Physics China, The Chinese Academy of Sciences, P.O. Box 2735, Beijing 100190, China

⁴Department of Electrical Engineering and Computer Science, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, USA

(Received 3 April 2017; revised manuscript received 30 June 2017; published 11 August 2017)

We theoretically investigate a novel and powerful double-pole nanoscale relay based on a carbon nanotube, which is one of the nanoelectromechanical switches being able to work under the strong nuclear radiation, and analyze the physical mechanism of the operating stages in the operation, including "pull in," "connection," and "pull back," as well as the key factors influencing the efficiency of the devices. We explicitly provide the analytical expression of the two important operation voltages, $V_{pull in}$ and $V_{pull back}$, therefore clearly showing the dependence of the material properties and geometry of the present devices by the analytical method from basic physics, avoiding complex numerical calculations. Our method is easy to use in preparing the design guide for fabricating the present device and other nanoelectromechanical devices.

DOI: 10.1103/PhysRevApplied.8.024006

I. INTRODUCTION

With the exponential growth in the number of devices in integrated circuits according to Moore's law [1], the size of semiconductor devices decreases and the power consumption of traditional semiconductor devices, such as complementary metal-oxide semiconductors (CMOS), increases correspondingly, and thus novel devices with low-power consumption are in high demand [2,3]. A nanoelectromechanical (NEM) switch is one of the promising candidates beyond CMOS [2,4-8], which takes advantage of the reduced leakage current, and therefore the reduced power consumption and the higher on:off ratio [4]. Moreover, nanoelectromechanical system (NEMS) switches have broad potential applications in extreme environments, such as in exploring aerospace and rescuing nuclear accidents, due to their tolerance to radiation [2], temperature variations [9], and external electric fields [10]. Recent studies demonstrate that nanoscale relays based on a carbon nanotube (CNT) have many potential applications, such as for logic devices, memory elements, and *I-V* amplifiers [7,8,11–18].

In a typical NEMS switch, the flexural beam deflects in response to an electrostatic force, and contact with the opposing electrode [2]. It is suggested that CNTs can work well as the flexural element in a NEMS switch, benefiting from the CNTs' unique elastic and electric properties [7,16]. In particular, a double-pole CNT nanoscale relay has been designed by Milaninia *et al.*, with a vertically grown CNT serving as an active switching element in response to an applied voltage so that its length is easy to be controlled [19]. This function is, in principle, easy to control in the fabrication process [11]. The operation of this CNT-based NEMS device is described as Fig. 1, and is featured by its two closed switching states, which can be switched to each other reversibly by an applied voltage. This present nanoscale relay makes use of an electrostatic interaction and of the elastic restoring force of the flexural beam by a mechanical deflection. Physically, the electrostatic force originates from the capacitor system consisting of the electrode and the active element.

The operation of the present nanoscale relay can be divided into three steps: "pull in," "connection," and "pull back," as shown in Fig. 1. At the pull-in process, with the increase of the voltage between the CNT and one electrode, an attractive electrostatic force leads to the bending of the CNT towards the electrode. At first, the deformed CNT keeps its equilibrium configuration in the motion since the electrostatic force and van der Waals (vdW) interaction can be balanced by the elastic restoring force. However, if $V > V_{\text{pull in}}$, the critical pull-in voltage, the balance breaks, the CNT bends dramatically and hits the electrode, which is a kind of electromechanical instability phenomenon [20–24]. At the connection stage, the curved CNT physically makes tight contacts with the electrode due to the short-range interatomic interaction between the carbon atoms in the CNT

muwh@itp.ac.cn

[†]Deceased.

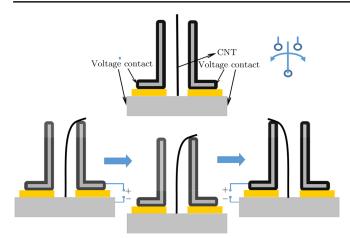


FIG. 1. Schematic sketch of a double-pole CNT nanoscale relay with a CNT in the center, between two electrodes, labeled voltage contacts. The CNT can switch to both electrodes in response to the applied voltage, and keep the closed state with the applied voltage withdrawn.

and the metal atoms in the electrode when the applied voltage is being withdrawn, as shown in Fig. 2. During the "pull-back" process, the voltage is applied across the CNT and the other electrode. If the voltage satisfies $V > V_{\text{pull back}}$, the critical voltage for pulling back, the flexural CNT separates from the other electrode, and moves towards the electrode and touches it, as shown in Fig. 2.

To optimize the design and the implementation of the present device described in this manuscript, we will accomplish this task by providing an analytical expression for the characteristic operation voltages of the present double-pole CNT nanoscale relay. We also investigate whether or not this double-pole CNT nanoscale relay

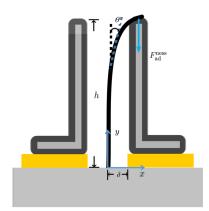


FIG. 2. Schematic sketch of the present double-pole CNT nanoscale relay designed by Milaninia [19] at the connection stage without an applied voltage. The CNT keeps touching the electrode by the adhesion force F_{ad} , which is assumed to be a perpendicular force. The contact point of the CNT and the electrode is assumed to be near the end of the CNT. The CNT is modeled as a bending hollow elastic rod with the θ measuring the bending of the centerline of the rod.

can function as a sub-one-volt device, and we discuss the relevant working parameters.

II. MODELING

A. Pull-in voltage of the double-pole CNT nanoscale relay

The pull-in response of the active element in the nanoscale relay is an instability phenomenon from the point of view of classical mechanical theory. It is, however, not the key point of our present work to make a highly detailed description of the instability phenomenon; rather, we aim to describe the pull-in voltage based on the simplest model with a minimal set of parameters. The model can correctly grasp the physical meaning of the pull-in operation of the present double-pole nanoscale relay, and provide the required pull-in voltage. In previous theoretical studies, most of the investigated nanoscale relays are one-point devices with only the pull-in voltage being the main characteristic of the devices [7,20-26]. Among these works on the experimental efforts of quantifying the pull-in behavior and modeling the dynamic pull-in instability, a typical theoretical work [25] studies the pull-in voltage of the CNT nanoscale relay using the lumped model and including a description of the competition between the electrostatic interaction (capacitive force of the active element-electrode system), the elastic energy of the continuum cantilever beam, as well as the van der Waals (vdW) interaction [25]. The theory is verified by moleculardynamics (MD) simulations [25]. The model is further developed by extending of the model containing additional effects, such as the Casimir forces [27], nonlocal elastic theory characterized by a complex stress-strain relation [28], and by including the effect of the concentration of electric charge at the end of the nanocantilever [29].

Here, we provide an analytical expression for the pull-in voltage of the present double-pole devices [19]. It is well known that the total vdW forces can be neglected, by comparing them with the elastic restoring force and the electrostatic force at $x \approx \delta/3$, the universal critical deformation of a cantilever for pull-in instability [25], leads only the lumped electrostatic force and an elastic restoring force on the CNT are important at the critical point of the pull-in instability. We suggest the simple expression of the pull-in operation voltage as the result of the competition between the restoring elastic force and the electrostatic attractive force [30],

$$V_{\text{pull in}} = \frac{2}{3} \frac{\delta}{L^2} \sqrt{\zeta/\eta} \sqrt{YI/\pi\epsilon_0 \epsilon_r} \ln\left(4\delta/3R_{\text{out}}\right). \quad (1)$$

Here, ζ and η are dimensionless quantities related to the geometry of the CNT, which is usually presented in the lumped component model of the electromechanical responses [7,25,26,31], describing the correction of the analytical expression due to the deflection of the central

active element; for example, ζ is 1–4 [7,25,26]. The *Y* and *I* in Eq. (1) are the Young's modulus and the second moment of area of the CNT, respectively. ϵ_0 is the permittivity of vacuum, and the ϵ_r is the relative permittivity of the medium in the gap between the two electrodes and the possibility of an air gap is also considered in our calculations. Obviously, all the present results can be easily extended to the non-air-gap case with a relative permittivity. The δ in Eq. (1) represents the distance of the gap shown in Fig. 2, and R_{out} is the radius of the CNT, which is the radius of the outer layer of the CNT with concentric cylindrical structure, as shown in Fig. 3.

Using a typical set of parameters, Y = 1TPa, $d_{in (out)} = 2.8 (3.5)$ nm, $\epsilon_r = 1$, and $\delta = 10$ nm, we obtain the relationship between $V_{pull in}$ and the length L of the CNT, as shown in Fig. 4. To verify the expression of pull-in voltage in Eq. (1), we compare our result with the result in Ref. [20], since the result of pull-in voltage in Ref. [20] has been verified by the experiments, and is comparable with the results by previous MD simulations [25]. The numerical results suggest our work is in good agreement with those in Ref. [20], which justifies the reasonability of our present result on pull-in voltage.

B. Mechanical balance of the CNT in the closed switch: Connection stage

After the pull-in operation, typically, the flexural element holds the contact of the CNT with the electrode by an adhesive force and keeps the circuit closed, even when the voltage is being withdrawn. To complete the following operation of pulling the CNT back to the other electrode (pull back), the adhesion at the interface of the electrode and the CNT is the key factor, which is, therefore, the important topic of the present study. The adhesive force F_{ad} results from the interatomic interaction between the CNT and the electrodes (see Fig. 2), which is usually studied by the MD method. However, the MD numerical computation for the interfacial interaction between a metal and carbon

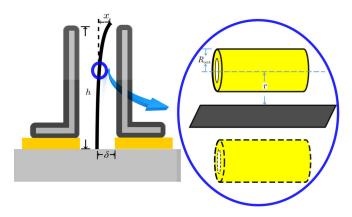


FIG. 3. Schematic drawing of calculation of capacitive force between the CNT and the conductive electrode by the electrostatic image method.

materials is usually highly time consuming and high in cost. In addition, using MD simulations, only systems with few atoms can be studied in an acceptable time under the present software and hardware conditions. The computation may possibly also encounter a finite size effect, leading to theoretical results that are not compatible with the operational behaviors of real devices. Moreover, the results of the MD simulation usually cannot be used conveniently for directing the fabrication of relevant devices. However, such calculations are useful to show the tendency of how the critical voltage changes in response to varying the pertinent parameters. In this manuscript, we study the working mechanism of the operations of the present double-pole device, and we provide analytical results, suggesting the dependence of main controlling parameters to the operational voltages, such as the material properties and aspect ratio of the devices. The results at present have the following simple forms, and can be easily used in finding the guiding rules for the manufacture of the present double-pole nanoscale relay device.

To maintain the contact, the relationship between the length of the rod *L* and the perpendicular adhesive force F_{ad}^{ness} necessary to maintain the balance of the torque, can be obtained by classical continuum elastic theory [30,32],

$$L = \sqrt{\frac{YI}{2F_{\rm ad}^{\rm ness}}} \int_0^{\theta_0} \frac{1}{\sqrt{\cos\theta - \cos\theta_0}} d\theta, \qquad (2)$$

which implies that

$$F_{\rm ad}^{\rm ness} = YI/L^2 f_1(\theta_0). \tag{3}$$

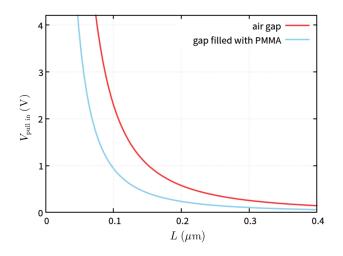


FIG. 4. The "pull-in" voltage for the present double-pole CNT nanoscale relay [19], with the DWCNT's diameters $d_{\rm in \ (out)} = 2.8 \ (3.5)$ nm, and the CNT length *L*. The DWCNT's Young's modulus is Y = 1.0 TPa, with dimensionless parameters $\zeta = 4$, and $\eta = 1$ [25], $\delta = 10$ nm is the gap distance. Red line, the air-gap case; blue line, the gap filled with a polymer PMMA with $\varepsilon_r = 6$.

Here, $\theta(l)$ is the angle between the tangent direction of the centerline of the rod and the vertical direction, as shown in Fig. 2, and $\theta(l)$ is introduced to describe the bending of the rod. The arc parameter of the curved CNT tube axis is $l \in (0, L)$. At the two ends of the rod, $\theta(0) = 0$, while $\theta(L) = \theta_0$ is to be determined self-consistently from Eq. (3). Here, $f_1(\theta_0)$ is a dimensionless factor to describe the θ_0 dependence of F_{ad}^{ness} on the CNT, which can be expressed by the incomplete elliptic integral of the first kind, F(k, l) [33], as [30]

$$f_1(\theta) = \csc^2\left(\frac{\theta_0}{2}\right) F^2\left[\csc\left(\frac{\theta_0}{2}\right), \frac{\theta_0}{2}\right].$$
 (4)

Here, "csc" denotes cosecant function. For simplicity, the adhesive force is assumed to be a perpendicular force exerted on the elastic rod, at the contact point, approximately at the end of the CNT, as shown in Fig. 2.

The elastic restoring force or torque depends on the deflection of the CNT, and the parametric expression of the center line of the rod, $\{x(\theta), y(\theta)\}, \theta \in (0, \theta_0)$, can be derived straightforwardly by [30]

$$x(\theta) = \int_0^\theta \sqrt{\frac{YI}{2F_{\rm ad}}} \frac{\sin\theta' d\theta'}{\sqrt{\cos\theta' - \cos\theta_0}},$$
 (5)

and

$$y(\theta) = \int_0^{\theta} \sqrt{\frac{YI}{2F_{\rm ad}} \frac{\cos \theta' d\theta'}{\sqrt{\cos \theta' - \cos \theta_0}}},$$
 (6)

which describes the bending of the CNT. The geometry of the device provides two constraint conditions: one is for δ , the width of the air gap, and the other is for h, the height of electrodes, as $x(\theta_0) = \delta$, and $y(\theta_0) = h$, assuming the contact point is closed to the end of the CNT. The contact angle θ_0 and the necessary adhesive force F_{ad}^{ness} on the CNT can be determined self-consistently from Eq. (3) and the constraint conditions for $x(\theta_0)$ and $y(\theta_0)$. Typically, the contact angle is small since $\delta/h \ll 1$ of the present double-pole device shown in Fig. 2, and $f_1(\theta_0) \approx 2$ in the small contact angle case, calculated from Eq. (4), thus $F_{ad}^{ness} \sim 2YI/L^2$ [30].

C. Adhesive force

As one of the passive forces, the adhesive force holding the CNT to the electrode is not a constant force. This adhesive force can vary from the zero-voltage value to the maximum value F_{ad}^{max} at the connection stage, in response to an increase of the force pulling the CNT back due to the elastic restoring force and electrostatic force. A simple expression with an analytical form of the adhesive force per unit area at he CNT/metal interface, derived from the Lennard-Jones potential, is enough for describing the short-range interaction, in order to demonstrate the mechanism of operations of the present double-pole devices [34],

$$p(d) = \frac{A}{6\pi d_0^3} \left[\left(\frac{d_0}{d} \right)^3 - \left(\frac{d_0}{d} \right)^9 \right],\tag{7}$$

where d is the distance between the surfaces of the CNT's outer carbon layer and the metal electrode, which is on the order of magnitude of an angstrom. The surface of the CNT and the metal electrode at the contact area is modeled as an effective planar surface. Here, the Hamaker constant $A \equiv 4\pi^2 \epsilon \rho_1 \rho_2 \sigma^6$ depends on the properties of the materials on both sides of the interface. In the Hamaker constant, ϵ and σ are the pair of parameters appearing in the Lennard-Jones potential shown in Eq. (7), which is the empirical potential widely used to describe the interaction between carbon atoms (in the CNT) and metal atoms (in the electrodes). The value of $d_0 = (2/15)^{1/6} \sigma \approx 0.7 \sigma$ is the equilibrium distance between the two surfaces corresponding to the minimum of the Lennard-Jones potential, and at this length scale, the CNT/electrode interface can be considered as a plane.

Since the adhesive force (per unit area) reaches its maximum at the distance $d_1 = 3^{1/6}d_0$, the maximal adhesive force is

$$F_{\rm ad}^{\rm max} = p_{\rm max} S_0$$
 and $p_{\rm max} = 3^{-5/2} A / \pi d_0^3$. (8)

The connection state without voltage is maintained, if the maximal adhesive force on the CNT, $F_{ad}^{max} = p_{max}S_0 \le F_{ad}^{ness}$. Here, S_0 , the contact area between the CNT and the electrode, can be adjusted by modifying the outer layer of the CNT, for example, by adding a patch of carbon material on the CNT [35].

To provide the pull-back voltage for the present doublepole nanoscale relay, we quantitatively study the adhesion effect between the electrode and the CNT. As an example, we consider the gold electrodes, and in this case, the Hamaker constant A becomes

$$A = 4\pi^2 \varepsilon_{\text{C-Au}} \rho_{\text{Au}} \rho_{\text{C}} \sigma_{\text{C-Au}}^6 \approx 0.14 \text{ eV}, \qquad (9)$$

with ρ the number density of the material in units of nm⁻¹, and $\rho_{Au} = 620 \text{ nm}^{-3}$, $\rho_C = 1.1 \times 10^3 \text{ nm}^{-3}$, $\varepsilon_{C-Au} = 2.2 \text{ meV}$, $\sigma_{C-Au} = 0.27 \text{ nm}$ [36]. The value of d_0 becomes $d_0 = (2/15)^{1/6} \sigma \approx 0.2 \text{ nm}$. The p(d) for a gold electrode reaches its maximum at $d_1 = (3^{1/6})d_0 = 0.24 \text{ nm}$, $p_{\text{max}} = p(d_1) = 3^{-5/2}A/\pi d_0^3 = 7.3 \text{ eV/nm}^3 = 1.2 \text{ nN nm}^{-2}$.

D. Mechanism of the pull-back operation

In the pull-back operation, the active element is switched towards the other electrode by applying a voltage between the curved CNT and the far-end electrode. To balance the varying torque generated by the electrostatic force, the

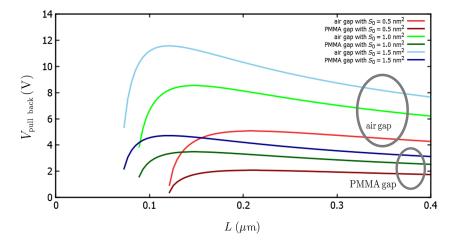


FIG. 5. Pull-back voltage $V_{\text{pull back}}$ for the present double-pole CNT nanoscale relay of CNT length *L* with a series of contact areas. The CNT serves as the active element of the nanoscale relay, which is modeled as a hollow rod of the circular cross section, with the inner (outer) diameter $d_{\text{in (out)}} = 2.8 (3.5)$ nm, to be in accordance with that in the CNT, the distance between the two adjacent carbon layers is 0.35 nm. As an estimation, the DWCNT's Young's modulus is approximately $Y \approx 1.0$ TPa, and the gap is $\delta = 10$ nm. The red lines denote the pull-back voltage for the CNT with a (effective) contact area $S_0 = 0.5$ nm², green lines denote the CNT relay with $S_0 = 1.0$ nm², and blue lines denote the system with $S_0 = 1.5$ nm², showing the importance of the contact area S_0 parameter. The upper group of red-green-blue curves are for the air-gap case, whereas the lower group are for the case of the gap filled with flexible polymer PMMA, manifesting the effect of the filling of the dielectric medium on the pull-back voltage.

interfacial adhesive force increases in response to the increasing voltage, until it reaches its extreme value F_{ad}^{max} . The torque balance at this critical state determines the pull-back voltage, and above the critical voltage $V > V_{pull back}$, the CNT is suddenly separated from the contacting electrode, and the device is then disconnected from the circuit. This process provides an on-off function to the circuit.

The electrostatic torque exerted on the whole CNT in the pull-back operation is calculated in a piecewise way, $dM_{\rm elec} = dF_{\rm elec}(y)y$, with the electrostatic force acting on the straight vertical piece of the CNT, and $dF_{\rm elec}(y) \approx \pi\epsilon_0 V^2 dy/[\delta + x(y)] \ln^2 \{2[\delta + x(y)]/R_{\rm out}\}$. The total electrostatic torque $M_{\rm elec}$ is, therefore,

$$\begin{split} M_{\text{elec}} &= \int_{0}^{h} \frac{\pi \epsilon_{0} \epsilon_{r} V^{2} y}{[\delta + x(y)] \ln^{2} \{ 2[\delta + x(y)] / R_{\text{out}} \}} \, dy \\ &\approx \int_{0}^{\delta - R_{\text{out}}} \frac{\pi \epsilon_{0} \epsilon_{r} V^{2}}{(x + \delta) \ln^{2} [2(x + \delta) / R_{\text{out}}]} \left(\frac{h}{\delta}\right)^{2} x dx \\ &= C_{1} \frac{h^{2}}{\delta} \pi \epsilon_{0} \epsilon_{r} V^{2}, \end{split}$$
(10)

where $C_1 = R_{out}[\text{li}(4\delta/R_{out}) - \text{li}(2\delta/R_{out})]/(2\delta) - 1/\ln(4\delta/R_{out})$, and li(z) is a logarithmic integral function [33,37].

In the present example, typical parameters for the air gap are $\delta = 10$ nm and $\epsilon_r = 1$. For simplification, a doublewalled carbon nanotube with inner (outer) diameters 2.8 (3.5) nm is considered, with a typical Young's modulus $Y \approx 1$ TPa. With the present set of parameters, the constant $C_1 \approx 0.03$ [30]. The corresponding torque of the electrostatic interaction is $M_{\rm elec} \approx C_1 (h^2/\delta) \pi \epsilon_0 \epsilon_r V^2 \propto V^2$, which depends on the aspect ratio $\gamma \equiv h^2/\delta$ of the device.

The torque of the interfacial force is $M_{\text{interfacial}} \approx (p_{\text{max}}S_0 - F_{\text{ad}})L$. At the critical state, the condition of the balance of the torques implies $M_{\text{interfacial}} = M_{\text{elec}} + M_{\text{vdW}} \approx M_{\text{elec}}$, since the van der Waals force is much smaller than the electrostatic force; therefore, we obtain

$$V_{\text{pull back}} \approx \sqrt{\frac{p_{\max}S_0 - 2YI/L^2}{C_1\pi\epsilon_0\epsilon_r}} \frac{\sqrt{L\delta}}{h}$$
$$\approx C_2 \sqrt{\frac{p_{\max}S_0 - 2YI/L^2}{L}}, \quad \text{and} \quad p_{\max}S_0 \ge F_{\text{ad}}, \tag{11}$$

in which $C_2 \equiv \sqrt{\delta/(\pi\epsilon_0\epsilon_r C_1)}$. Here, we have used the fact that $\delta \ll h \approx L$ to simplify the writing of our result. The theoretical results of Eq. (11) are shown in Fig. 5, in the plot of $V_{\text{pull back}}$ vs L, the length of the CNT. These calculated results imply that the CNT nanoscale relay shown in Fig. 2 should be carefully designed to make sure that the device is working within the small voltage region. Typically, the pull-in voltage can be less than 1V for the present two-pole CNT nanoscale relay to be able to be switched back and forth, if the pull-back voltage is larger than the pull-in voltage. For a rough estimation of the present nanoscale relay based on a CNT, a double-walled carbon nanotube (DWCNT) is modeled as a hollow elastic rod of circular cross section, with the thickness of the rod's wall being 0.35 nm, which is in accordance with the distance between the two adjacent carbon layers in a DWCNT. To simplify, we use an inner (outer) diameter $d_{in (out)} = 2.8 (3.5)$ nm. The air gap is set to be $\delta = 10$ nm. This result implies that the pull-back voltage depends on the length of the CNT, the contact area between the CNT and the electrode, the material properties of the CNT and the electrodes, as well as the device's aspect ratio $\gamma = h/\delta$. Here, as an example, we consider a gold electrode. To make the real device operate, the outer carbon layer of the contact area of the CNT can be modified to adjust the adhesive force. The elastic properties of the CNT are characterized by the product of the Young's modulus Y and I the second moment of area, YI. The working voltage of the CNT nanoscale relay can be designed by carefully tuning the related parameters to obtain the voltage $V_{\text{pull back}}$ by the nanotube length L, as shown in Fig. 5. To make the double-pole nanoscale relay work, $p_{\text{max}}S_0 \ge 2YI/L^2$ implies that there is an upper bound for the ratio $R_{\rm out}/L$, since that $S_0 \propto R_{out}$, and $I \propto R_{out}^3$ with the assumption that the thickness of CNT is much less than the diameter of the outer wall of CNT. This provides a restriction on the geometrical parameters of the present double-pole CNT nanoscale relay.

III. DISCUSSION

In our theoretical modeling and calculation, the key point is the study of the importance of the adhesive force between the outer surface of the CNT and the metal electrode. We consider the physical absorption effect, which is due to the short-range interatomic interaction, without an electron transfer across the interface. Based on this assumption, we use the well-established adhesive force theory based on the Hamaker constant [34]. Microscopically, the interaction between the CNT and the electrode is the adhesion between the two surfaces which are close to each other, and the adhesive force per unit area is described by Eq. (7). For very smooth surfaces, the chemisorption may become important, and this force is related to the electron transfer between the carbon atoms and the metal atoms in the electrode [38]. In addition, the adhesion can be adjusted by a chemical modification of the surfaces. This technique, together with controlling the contact area, can effectively adjust the pull-back voltage to make the device work under various operating conditions to comply with the industrial standards for electronic devices.

To lower the working voltage, we propose a gap filled with the polymer with the higher dielectric permittivity in the device, instead of the air gap. For simplification, we do not consider the resistance to the active element during the operations, caused by the polymer, due to our assumption of the loose padding. This effect may provide a small correction factor, and will be studied in the research to follow. In the studies of the electromechanical response of devices based on a CNT, the charge distribution in the CNT under the electrostatic field is important; for example, the phenomenon of the charge concentration at the free end of the CNT discussed in Ref. [29] leads to an observable effect. We will address this effect in the work to follow.

In summary, we establish a generic model for a type of double-pole CNT nanoscale relay with high nuclear radiation tolerance originally proposed by Milaninia *et al.* [19]. We quantitatively analyze the function and operation of our version of the device concept. We theoretically obtain the analytical expressions for the critical voltages for the pull-in and pull-back operations, from the basic physics, which strongly depend on the materials properties of the CNT relay system. The numerical results obtained here are in reasonable agreement with relevant experimental reports reviewed in the recent literature [2]. The model can be used to predict phenomena in future experiments on NEMS and to improve designs for the nanoscale relay based on a CNT.

ACKNOWLEDGMENTS

Z.-c. O.-Y. thanks the National Basic Research Program of China (973 program, No. 2013CB932804); and the Joint NSFC-ISF Research Program, jointly funded by the National Natural Science Foundation of China and the Israel Science Foundation (No. 51561145002) for financial support. W. M. and Z.-c. O.-Y. thank the National Science Foundation of China (NSFC), Grant No. 11374310. M. S. D. acknowledges support from the U.S. NSF, Grant No. DMR-1507806.

APPENDIX: DETAILS OF OBTAINING THE "PULL-IN" VOLTAGE

For simplicity, the double-wall CNT is used in the present calculations, which is modeled as a circular cross-sectional hollow rod. The elastic energy of a curved CNT can be written as $E_{\text{elas}} \approx \zeta(YI/L^3)x^2$, with *x* being the horizontal displacement of the end of the curved CNT, $Y \approx 1$ TPa being the typical Young's modulus of a CNT, and the rod's second moment of area given by $I = \pi (d_2^4 - d_1^4)/64$, with an inner (outer) diameter of the double-wall nanotube being $d_{1(2)} = 2R_{\text{in (out)}}$, $(R_{\text{in (out)}})$, the radii of the carbon layers in CNT, respectively. Here, the model-dependent dimensionless parameter ζ is introduced into the elastic energy of the CNT $E_{\text{elas}} \propto x^2$. For a cantilever-beam-like active element, $\zeta = 4$ [25], $\zeta = 3/2$ [7], and $\zeta = 1.6$ [26] are different values calculated by different models [7,25,26].

The electrostatic energy of the CNT nanoscale relay can be obtained from a classical theory of the capacitive energy of a CNT-electrode capacitor system. The capacitance per unit length of the system is approximately [25]

$$c(r) = \frac{2\pi\epsilon_0}{\ln\left(\sqrt{r^2/R_{\text{out}}^2 - 1} + r/R_{\text{out}}\right)},\qquad(A1)$$

which is derived from the electrostatic image method [39], as shown in Fig. 3. Here, r is the distance between the axis of the CNT and the planar surface of the electrode. The electrostatic energy can be written as

$$E_{\text{elec}} \approx \frac{1}{2} \eta V^2 c(\delta - x)$$

= $\eta V^2 \frac{\pi \epsilon_0 \epsilon_r}{\ln \left[\sqrt{(\delta - x)^2 / R_{\text{out}}^2 - 1} + (\delta - x) / R_{\text{out}}\right]}.$ (A2)

Here, η is a dimensionless parameter denoting the correction due to the bending of the CNT, and the meaning of *x* is the same as that in the elastic energy expression.

The competition between the capacitive force and the elastic force determines the pull-in instability, which can be obtained from the derivative of the corresponding energy $\partial E_{\text{elas (elec)}}/\partial x$, for example, to obtain $F_{\text{elas}} = 2\zeta (YI/L^3)x$. The balance of the elastic restoring force and the electrostatic force at the critical deflection $x_c \approx \delta/3$ determines the pull-in voltage.

- G. E. Moore, Cramming more components onto integrated circuits, Electronics 38, 114 (1965); http://ieeexplore.ieee .org/stamp.jsp?arnumber=4785860.
- [2] O. Y. Loh and H. D. Espinosa, Nanoelectromechanical contact switches, Nat. Nanotechnol. 7, 283 (2012).
- [3] A. Peschot, C. Qian, and T-J. K. Liu, Nanoelectromechanical switches for low-power digital computing, Micromachines 6, 1046 (2015).
- [4] S. W. Lee, S. J. Park, E. E. B. Campbell, and Y. W. Park, A fast and low-power microelectromechanical system-based non-volatile memory device, Nat. Commun. 2, 220 (2011).
- [5] Y. H. Chen, R. Nathanael, J. Yaung, L. Hutin, and T.-J. K. Liu, Reliability of MEM relays for zero leakage logic, Proc. SPIE Int. Soc. Opt. Eng. 8614, 861404 (2013).
- [6] J. O. Lee, Y-H. Song, M-W. Kim, M-H. Kang, J-S. Oh, H-H. Yang, and J-B. Yoon, A sub-1-volt nanoelectromechanical switching device, Nat. Nanotechnol. 8, 36 (2013).
- [7] J. M. Kinaret, T. Nord, and S. Viefers, A carbon-nanotubebased nanorelay, Appl. Phys. Lett. 82, 1287 (2003).
- [8] S. W. Lee, D. S. Lee, R. E. Morjan, S. H. Jhang, M. Sveningsson, O. A. Nerushev, Y. W. Park, and E. E. B. Campbell, A three-terminal carbon nanorelay, Nano Lett. 4, 2027 (2004).
- [9] T-H. Lee, S. Bhunia, and M. Mehregany, Nanoelectromechanical computing at 500 °C with silicon carbide, Science 329, 1316 (2010).
- [10] L. M. Jonsson, S. Axelsson, T. Nord, S. Viefers, and J. M. Kinaret, High frequency properties of a CNT-based nanorelay, Nanotechnology 15, 1497 (2004).

- [11] 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, Nanoelectromechanical switches with vertically aligned carbon nanotubes, Appl. Phys. Lett. 87, 163114 (2005).
- [12] T. Rueckes, K. Kim, E. Joselevich, G. Y. Tseng, C. L. Cheung, and C. M. Lieber, Nanoelectromechanical switches with vertically aligned carbon nanotubes, Science 289, 94 (2000).
- [13] W. Xiang and C. Lee, Nanoelectromechanical torsion switch of low operation voltage for nonvolatile memory application, Appl. Phys. Lett. 96, 193113 (2010).
- [14] Q. Li, S-M. Koo, M. Edelstein, J. Suehle, and C. Richter, Silicon nanowire electromechanical switches for logic device application, Nanotechnology 18, 315202 (2007).
- [15] K. J. Ziegler, D. M. Lyons, J. D. Holmes, D. Erts, B. Polyakov, H. Olin, K. Svensson, and E. Olsson, Bistable nanoelectromechanical devices, Appl. Phys. Lett. 84, 4074 (2004).
- [16] O. Loh, X. Wei, C. Ke, J. Sullivan, and H. Espinosa, Robust carbon nanotube based nanoelectromechanical devices: Understanding and eliminating prevalent failure modes using alternative electrode materials, Small 7, 79 (2011).
- [17] J.-W. Han, J.-H. Ahn, M.-W. Kim, J. O. Lee, J.-B. Yoon, and Y.-K. Choi, Nanowire mechanical switch with a built-in diode, Small 6, 1197 (2010).
- [18] J. E. Jang, S. N. Cha, Y. J. Choi, D. J. Kang, T. P. Butler, D. G. Hasko, J. E. Jung, J. M. Kim, and G. A. J. Amaratunga, Nanoscale memory cell based on a nanoelectromechanical switched capacitor, Nat. Nanotechnol. 3, 26 (2008).
- [19] K. Milaninia, T. Akinwande, and M. Baldo (private communication).
- [20] C. Ke, N. Pugno, B. Peng, and H. D. Espinosa, Experiments and modeling of carbon nanotube-based NEMS devices, J. Mech. Phys. Solids 53, 1314 (2005).
- [21] C. Ke and H. D. Espinosa, Numerical analysis of nanotubebased NEMS devices—Part I: Electrostatic charge distribution on multiwalled nanotubes, J. Appl. Mech. 72, 721 (2005).
- [22] C. Ke, H. D. Espinosa, and N. Pugno, Numerical analysis of nanotube-based NEMS devices—Part II: Role of finite kinematics, stretching and charge concentration, J. Appl. Mech. 72, 726 (2005).
- [23] C. Ke and H. D. Espinosa, *In situ* electron microscopy electromechanical characterization of a bistable NEMS device, Small 2, 1484 (2006).
- [24] C. Ke, Resonant pull-in of a double-sided driven nanotubebased electromechanical resonator, J. Appl. Phys. 105, 024301 (2009).
- [25] M. Dequesnes, S. V. Rotkin, and N. R. Aluru, Calculation of pull-in voltages for carbon-nanotube-based nanoelectromechanical switches, Nanotechnology 13, 120 (2002).
- [26] S. Bhunia, M. Tabib-Azar, and D. Saab, in *Proceedings* of the Asia and South Pacific Design Automation Conference (ASP-DAC), Yokohama, Japan (IEEE, New York, 2007), p. 383; http://ieeexplore.ieee.org/stamp/ stamp.jsp?arnumber=4196001.
- [27] W-H. Lin and Y-P. Zhao, Stability and bifurcation behaviour of electrostatic torsional NEMS varactor influenced by dispersion forces, J. Phys. D 40, 1649 (2007).
- [28] J. Yang, X. L. Jia, and S. Kitipornchai, Pull-in instability of nano-switches using nonlocal elasticity theory, J. Phys. D 41, 035103 (2008).

- [29] C. Ke and H. D. Espinosa, Feedback controlled nanocantilever device, Appl. Phys. Lett. 85, 681 (2004).
- [30] See Supplemental Material at http://link.aps.org/ supplemental/10.1103/PhysRevApplied.8.024006 for more information on the details of deriving.
- [31] J. A. Pelesko and D. H. Bernstein, *Modeling MEMS and NEMS* (Chapman & CRC, London, 2002), p. 229.
- [32] L. Landau and E. Lifshitz, *Theory of Elasticity*, 3rd ed. (Pergamon Press, London, 1985).
- [33] M. Abramowitz and I. Stegun, *Handbook of Mathematical Functions*, 9th printing (Dover Publications, Inc., New York, 1972).
- [34] N. Yu and A. A. Polycarpou, Adhesive contact based on the Lennard-Jones potential: A correction to the value of the equilibrium distance as used in the potential, J. Colloid Interface Sci. 278, 428 (2004).

- [35] Y. H. Kahng, J. Choi, B. C. Park, D-H. Kim, J.-H. Choi, J. Lyou, and S. J. Ahn, The role of an amorphous carbon layer on a multiwall carbon nanotube attached atomic force microscope tip in making good electrical contact to a gold electrode, Nanotechnology 19, 195705 (2008).
- [36] S. Arcidiacono, J. H. Walther, D. Poulikakos, D. Passerone, and P. Koumoutsakos, Solidification of Gold Nanoparticles in Carbon Nanotubes, Phys. Rev. Lett. 94, 105502 (2005).
- [37] I. S. Gradshteyn and I. M. Tyzhik, *Table of Integrals, Series and Products*, 7th ed. (Elsevier Pte Ltd., Singapore, 2007).
- [38] C. W. Padgett and D. W. Brenner, Influence of chemisorption on the thermal conductivity of single-wall carbon nanotubes, Nano Lett. 4, 1051 (2004).
- [39] J. D. Jackson, *Classical Electrodynamics*, 3rd ed. (John Wiley & Sons, New York, 1998).