# Molecular Dynamics Study of Electromechanical Nanotube Random Access Memory

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## ABSTRACT

A nanoelectromechanical (NEM) switching device based on carbon nanotube (CNT) was investigated using atomistic simulations. The model schematics for a CNT-based three-terminal NEM switching device fabrication were presented. For the CNT-based three-terminal NEM switch, the interactions between the CNT-lever and the drain electrode or the substrate were very important. When the electrostatic force applied to the CNT-lever was the critical point, the CNT-lever was rapidly bent because of the attractive force between the CNT-lever and the drain; then, the total potential energy of the CNT-lever was rapidly increased and the interatomic potential energy of the CNT-copper was rapidly decreased. The energy curves for the pull-in and the pull-out processes showed the hysteresis loop that was induced by the adhesion of the CNT on the copper, which was the interatomic interaction between the CNT and the copper.

***Keywords***: nanoelectromechanical switch, carbon nanotube, nanorelay, three-terminal switch, molecular dynamics simulation

## 1 INTRODUCTION

Microelectromechanial systems (MENS) have already had a significant impact on medical, automobile, aerospace, and information technology areas [1]. Nanoelectromechnical systems (NEMS) are about a thousand times smaller than MEMS and have the potential to enable revolutionary technology for various areas. Hierold [2] discussed that microsystems will go nanosystems provided that self-assembly of nanostructure becomes a will-controlled fabrication technology. To date, NEMS are rapidly growing area of research with considerable potential for future applications [3]. The basic idea underlying NEMS is the strong electromechanical coupling in devices on the nanometer scale in which the Coulomb forces associated with device operation are comparable with the chemical binding forces.

Carbon nanotubes (CNT) [4] are excellent candidates for NEMS devices not only because of their excellent electronic and mechanical properties, but also because of the significant progress that have been made in the last few years in fabrication of carbon nanostructures [5]. This is a consequence of their well-characterized chemical and physical structures, low mass and dimensions, exceptional directional stiffness, and range of electronic properties [6]. Several possible devices based on CNTs have been investigated: nano-bearings [7-9], nano-gears [10,11], constant-force nano-springs [12], mechanical nano-switch [13], electrical nano-switch and nano-drill [14], gigahertz oscillators [15-19], data storage nano-devices [20-22], etc.

Some prototype CNT-based NEMS have already been demonstrated, such as nanotweezers [23], a random access memory [24], and sensors [25]. Recently the two-terminal CNT switch [26] and the three-terminal CNT nanorelay [27-29] have been studied theoretically. The nanorelay was shown theoretically to act as a switch in the GHz regime and to be potentially suitable for applications such as logic devices, memory elements, pulse generators, and current or voltage amplifiers [28].

However, the analysis of the impact of short-range forces on device design and performance has never been discussed in the previous works. Another effect including the possibility of field emission has been neglected. In this paper, we show model schematics for a three-terminal nanoelectromechancial (NEM) switch and then also perform classical molecular dynamics simulations for the NEM switch.

## 2 MODEL SCHEMATICS

Figure 1 shows the model schematics for a CNT-based NEM switching device fabrication. After the oxide film growth on the substrate (Fig. 1(a)), the gate electrode is formed as shown in Fig. 1(b). The drain electrode is also formed on the substrate as shown in Fig. 1(c). Another oxide film is also grown (Fig. 1(d)), and a CNT is deposited on the oxide film as shown in Fig. 1(e). The source electrode is deposited to cover one-side of the CNT (Fig. 1(f)). Finally, when the second oxide film is removed by the oxide etching processes in the condition that the etching gases cannot affect the CNT, the NEM switching device called the nanorealy can be fabricated as shown in Fig. 1(g). A conducting CNT is connected to a source electrode and suspended above the surface of a substrate, above gate and drain electrodes. The key components are a movable CNT as switching bar, a gate electrode for position control of the

movable CNT, and a drain electrode. Electrical charge is induced in the suspended CNT by a voltage applied to the gate electrode. The resulting capacitive force between the CNT and the gate bends the CNT and brings the CNT end into electrical contact with the drain electrode.

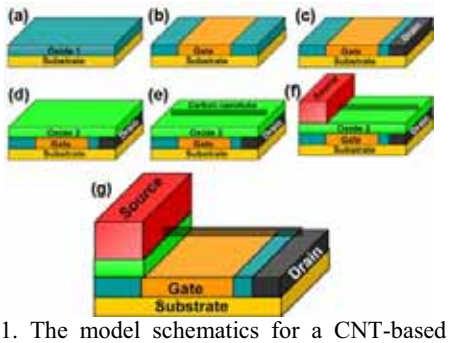


Figure 1. The model schematics for a CNT-based NEM switching device fabrication. (a) Oxide film growth on the substrate, (b) gate electrode formation, (c) drain electrode formation, (d) another oxide film growth, (e) CNT deposition on the oxide film, (f) source electrode formation to cover one-side of the CNT, and (g) finally, the second oxide film removal.

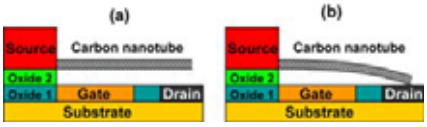


Figure 2. The physical operation of a CNT-based NEM switch. (a) Turn-on and (b) turon-off states.

Figure 2 shows the physical operation of a CNT-based NEM switch. When the potential different is achieved between the CNT and the gate electrode and between the CNT and the drain electrode, electrostatic charges are induced on both the CNT and the electrodes. The electrostatic charges give rise to electrostatic force, which deflect the CNT. In addition to electrostatic forces, depending on the gap between the CNT and the electrodes, the interatomic interactions also act on the CNT and deflect the CNT. The electrostatic and the interatomic forces make the CNT to bend toward the drain. Counteracting the electrostatic and interatomic forces are elastic forces, which try to restore the CNT to its original straight position. For an applied voltage, an equilibrium position of the CNT is defined by the balance of the elastic, electrostatic, and interatomic forces.

When the applied potential difference between the CNT and the gate electrode exceeds a certain potential, the CNT becomes unstable and collapses onto the substrate. The potential difference, which causes the CNT to contact onto the drain, is defined as the pull-in voltage. When the pull-in voltage is applied, the CNT comes in contact with the drain electrode, and the device is said to be in the ON state (shown in Fig. 2(b)). When the potential is released and the CNT and the drain electrode are separated, the device is said to be in the OFF state (shown in Fig. 2(a)).

Due to the exponential dependence of the tunneling resistance on tube deflection, there is a sharp transition from a non-conducting (OFF) to a conducting (ON) state when the gate voltage is varied at fixed source-drain voltage. The sharp switching curve allows for amplification of weak signals superimposed on the gate voltage.

## 3 MODEL STRUCTURE AND INTERATOMIC POTENTIALS

For C-C interactions, we used the Tersoff-Brenner potential function that has been widely applied to C systems [31-33]. The long-range interactions were characterized with the Lennard-Jones 12-6 (LJ12-6) potential that was continually connected by the cubic spline functions with the Tersoff-Brenner potential such as methods by Mao *et al* [39] when the interatomic distance ($r$) is between 2.0 and 2.7 Å. The cutoff distance of the LJ12-6 with parameters $\varepsilon_C = 0.0024$ eV and $\sigma_C = 3.37$ Å was 10 Å. We assumed the Cu nanowires as the conductor material. For Cu–Cu and Cu–C, we used the Mores-type potential, a pair interatomic potential function, which have been widely used in many atomistic studies for nanoindentations and nanomechanics [34,35].

The MD simulations used the same MD methods as were used in our previous works [36,37]. The MD code used the velocity Verlet algorithm, and neighbor lists to improve computing performance. MD time step was $5\times10^{-4}$ ps. A Gunsteren-Berendsen thermostat was used to control temperature for all atoms except for fullerenes. The structure was initially relaxed by the steepest descent method; then the atoms of both edges were fixed during the MD simulations and on the other atoms, MD methods were applied.

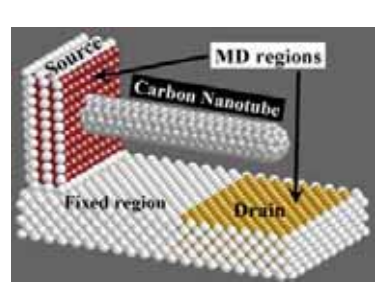


Figure 3. The atomic structure for the three-terminal NEM switching device. This structure is the same as the structure of Fig. 3 except for the substrate including drain electrode. The substrate was composed of 2400 copper atoms in $26\times70\times12$ Å$^3$. The drain region was 50 to 70 Å of the substrate.

Figure 3 shows the atomic structure for the three-terminal NEM switching device. The length of the (5,5) CNT was approximately 60 Å. The (100) copper surface acting as the source electrode for the three-terminal switch device was composed of 663 atoms, 26 Å$\times$26 Å$\times$9 Å. The

CNT is inserted at the center of the copper surface; then, the 9 Å of the CNT overlapped the copper surface. The substrate was composed of 2400 copper atoms, 26 Å × 70 Å × 12 Å. The boundary layers of the copper were fixed in the MD simulations and the other copper atoms were under the constraint dynamics to a constant temperature in the MD simulations. Ten carbon atoms of the bottom were fixed during the MD simulations but the other carbon atoms were applied to free MD simulations without any constraint dynamics. The drain region was 50 to 70 Å of the substrate. Copper atoms composed of the substrate except for the drain region were fixed in the MD simulations. The height of the CNT was 18 Å higher than the substrate.

## 4 RESULTS AND DISCUSSION

We investigated a three-terminal switch of the CNT-lever shown in Fig. 3 using the SD and the MD simulations. For the three-terminal switching devices, which have investigated by theoretical methods and by experimental methods, the interaction between the CNT-lever and the drain electrode or the substrate is very important. Dequesnes et al. [26] investigated the significance of the vdW interactions in the design of the two-terminal NEM switches. Kinaret et al. [27] investigated the three-terminal NEM switch using a simple model and discussed the characteristics of the device. Ke and Espinosa [28] developed the model for the switchable CNT-lever device including the concentration of electrical charge and the vdW force. Jonsson et al. [29] showed that the short range and the vdW forces have a significant impact on the characteristic of the three-terminal NEM switch. Therefore, for the three-terminal NEM switch as shown in Fig. 4, the significance of the interaction between the CNT-lever and the drain electrode was investigated using the SD and the MD simulations.

Figure 4 shows the pull-in of the three-terminal NEM switch using the SD simulation. We calculated the total potential energy of the CNT-copper interactions (Fig. 4(a)) and the total potential energy of the CNT (Fig. 4(b)) as a function of the external force per atom. The three snapshots in Fig. 4 show the atomic structures corresponding to the indicated external forces. The interatomic potential energy between the CNT and the source is –21.95 eV. The interatomic potential energy between the CNT and the drain is –16.11 eV when the CNT-lever is fully contacted with the drain. When the external force per atom is 0.0014 eV/Å, the CNT-lever is rapidly bent because of the attractive force between the CNT-lever and the drain; then, the total potential energy of the CNT-lever is rapidly increased and the total potential energy of the CNT-copper is rapidly decreased. Therefore, the long range or the short range interactions between the CNT-lever and the metal electrode are very important for the three-terminal NEM switch to operate such as the investigations of the previous papers.

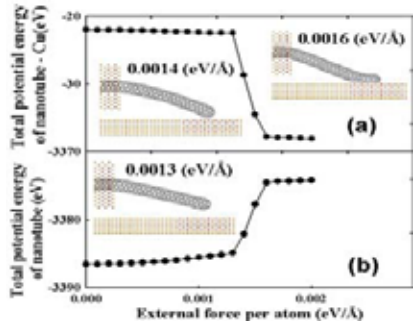


Fig. 4. The pull-in of the three-terminal NEM switch using the SD simulation. (a) The total potential energy of the CNT-copper interactions and (b) the total potential energy of the CNT as a function of the external force per atom. The three snapshots show the atomic structures corresponding to the indicated external forces.

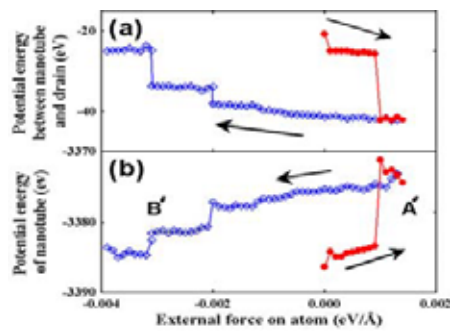


Fig. 5. The MD simulation results for the pull-in and the pull-out of the CNT-lever. (a) and (b) show the potential energies of the CNT-drain interaction and the CNT, respectively. The pull-in force increased from 0 to 0.0014 eV/Å and the pull-out force decreased to –0.0039 eV/Å

We performed the MD simulation for the pull-in and the pull-out of the CNT-lever as shown in Fig. 5. Figures 5(a) and 5(b) show the potential energies of the CNT-drain and the CNT, respectively. The pull-in force increased from 0 to 0.0014 eV/Å and the pull-out force decreased to –0.0039 eV/Å. When the external force per atom was 0.001 eV/Å, the CNT-lever contacted with the drain. The pull-in force for the switch turn-on was above 0.001 eV/Å per atom. In the MD simulation for the pull-out of the CNT-lever, three stages are found such as full-contacting, edge-contacting, and non-contacting. Figure 6(a) and 6(b) indicate the structures corresponding to the labels A' and B' in Fig. 5 (b). Figures 6(a) and 6(b) show the full contacting and the edge-contacting modes. In the pull-out simulations, the full contacting mode is until –0.0019 eV/Å, the edge-contacting mode is –0.002 to –0.0031 eV/Å, and the non-contacting mode is below –0.0032 eV/Å. Therefore, the pull-out force for the switch turn-off is below –0.0032 eV/Å. The energy curves for the pull-in and the pull-out processes show the hysteresis loop shown in Fig. 5. The difference between the turn-on and the turn-off forces, called the hysteresis loop, is

induced by the adhesion of the CNT on the copper, which is the interatomic interaction between the CNT and the copper. The hysteresis loop has been found in the previous theoretical works [27-29] and the previous experimental work [30]. This difference in the hysteresis loop makes the three-terminal NEM switch device to utilize a memory device [28].


Fig. 6. (a) and (b) indicate the structures corresponding to the labels A' and B' in Fig. 12 (b).

## 5 SUMMARY

We investigated a nanoelectromechanical (NEM) switching device based on carbon nanotube (CNT) using atomistic simulations. We presented the model schematics for a CNT-based three-terminal NEM switching device fabrication. The CNT-based NEM switch should be operated when the electrostatic force acting on the CNT-lever is below the critical point. The electrical-induced potential energy was changed to the mechanical energy. For the CNT-based three-terminal NEM switch, the interaction between the CNT-lever and the drain electrode or the substrate was very important. When the external force per atom was the critical point, the CNT-lever was rapidly bent because of the attractive force between the CNT-lever and the drain; then, the total potential energy of the CNT-lever was rapidly increased and the total potential energy of the CNT-copper was rapidly decreased. The energy curves for the pull-in and the pull-out processes showed the hysteresis loop that was induced by the adhesion of the CNT on the copper, which was the interatomic interaction between the CNT and the copper. The three-terminal NEM switch device could be applied to a memory device because of the difference in the hysteresis loop. For various materials for the drain, the operating properties of the NEM switch should be investigated in further works.

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