A Study of Electromechanical Nanotube Memory Device using Molecular Dynamics

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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. 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.

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. 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) [2] 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 [3]. Several possible devices based on CNTs have been investigated: nano-bearings [4], nano-gears [5], constant-force nano-springs [6], mechanical nano-switch, electrical nano-switch and nano-drill, gigahertz oscillators [7], data storage nano-devices [8.9], etc. 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. MODELING AND INTERATOMIC POTENTIALS

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.

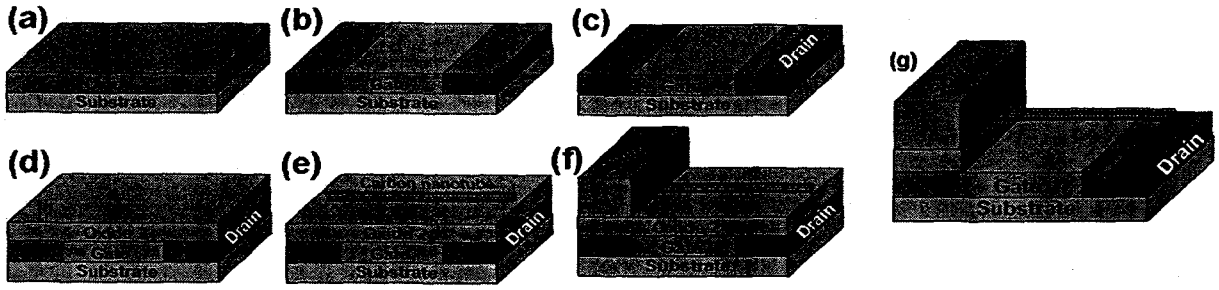

Fig. 1. The model schematics for a CNT-based NEM switching device fabrication.

For C-C interactions, we used the Tersoff-Brenner potential function that has been widely applied to C systems [10]. 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* [11] when the interatomic distance (r) is between 2.0 and 2.7 Å. The cutoff distance of the LJ12-6 with parameters ε_c= 0.024eV and σ_c= 37 . 3 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 [12]. The MD code used the velocity Verlet algorithm, and neighbor lists to improve computing performance. MD time step was 5×10^{-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.

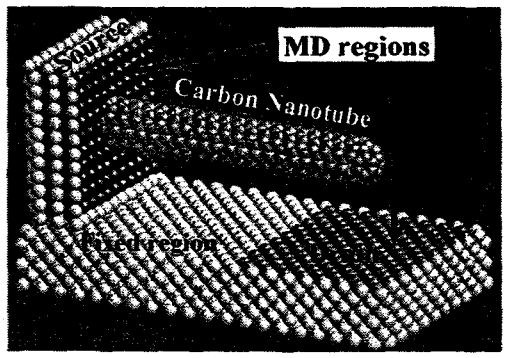

Fig. 2. The atomic structure for the three-terminal NEM switching device.

Figure 2 shows the atomic structure for the threeterminal 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 × 26 Å × 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.

3. RESULTS AND DISCUSSIONS

Figure 3 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. 3(a)) and the total potential energy of the CNT (Fig. 3(b)) as a function of the external force per atom. The three snapshots in Fig. 3 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. We performed the MD simulation for the pull-in and the pull-out of the CNT-lever as shown in Fig. 4. Figures 4(a) and 4(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.

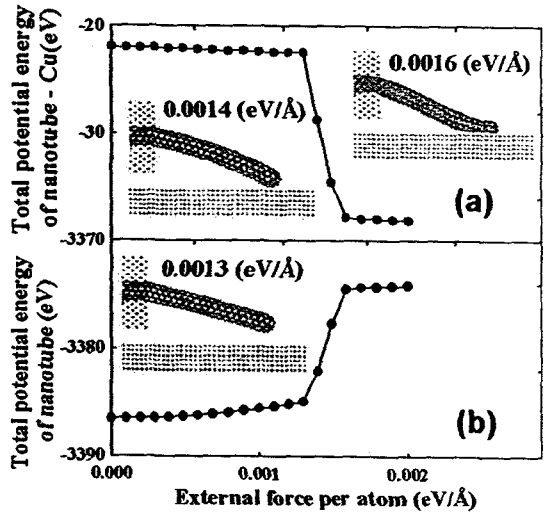

Fig. 3. The pull-in of the three-terminal NEM switch using the SD simulation.

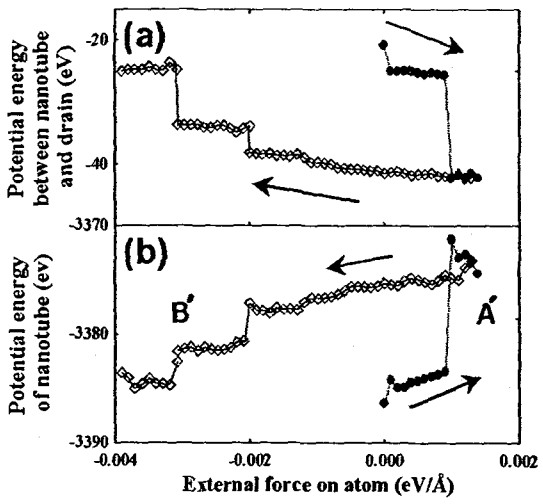

Fig. 4. The MD simulation results for the pull-in and the pull-out of the CNT-lever.

Figure 5(a) and 5(b) indicate the structures corresponding to the labels A' and B' in Fig. 4 (b). Figures 5(a) and 5(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. 4. 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.

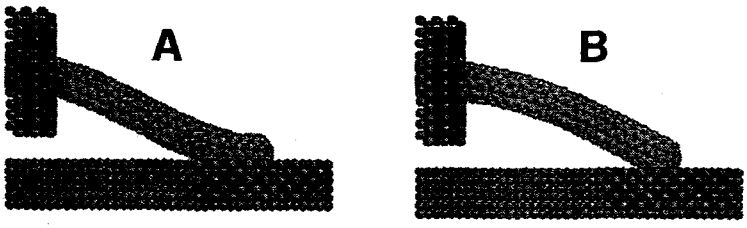

Fig. 5. (a) and (b) indicate the structures corresponding to the labels A' and B' in Fig. 4 (b).

4. CONCLUSIONS

We investigated a NEM switching device based on 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 CNTlever 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. 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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