Molecular Dynamics Simulations of Nonvolatile Carbon Nanotube Shuttle Memory


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ABSTRACT

We propose a novel carbon-nanotube (CNT)-based nonvolatile memory, which can serve as a key building block for molecular-scale computers and perform molecular dynamics simulations to investigate the dynamic operations of a double-walled CNT memory. We find that the most important physical characteristics of the proposed nanometer-scale memory device are the bi-stability achieved by both the CNT inter-wall vdW der Waals interaction and CNT-metal binding energies and the reversibility by electrostatic attractive forces. Since the CNT shuttle can have a high kinetic energy during the transition, the dynamical collisions between the CNT and the metal electrodes are very important factors to be considered for design of the electrostatically telescoping CNT memory. The long collision time and the several rebounds cause a delay of the state transition.

Keywords: molecular dynamics, carbon nanotube, nonvolatile memory

1 INTRODUCTION

Nanostructures such as quantum dots, nanowires and carbon nanotubes (CNTs) possess unique properties that make them promising candidates for future technology applications, due to their low dimensionality. Possibly a more promising candidate as a building block for molecular electronics and data storage is the CNTs [1], hollow tube-like molecule composed of carbon atoms closed on both ends, which have been widely experimented with and analyzed for their potential as an important new material in future micro- and nanoelectronics. CNTs also present a unique opportunity as one of the few systems where atomistic based modelling may reach the experimental device size, thus in principle allowing the experimental testing of computational approaches and computational device design. While similar approaches are under development for nanoscale silicon devices, the much different properties of CNTs require an entirely separate field of research. Despite substantial theoretical advantages of these modern approaches, currently proposed technologies are complicated and not yet matured for manufacture and mass production [2-8]. Thus, attempts to propose concepts and develop new types of nanomemory continue.

In this paper, we investigate a macroscopically addressable data storage device based on CNTs, which can be utilized both as nonvolatile random access memory and terabit solid-state storage. We present the conceptual design for such a device based on telescoping a MWCNT, and we study its dynamic characteristics using molecular dynamics (MD) simulations.

2 CONCEPTUAL DESIGN

A conceptual design and the operation principle of a MWCNT-based storage or nonvolatile memory are illustrated in figures 1 and 2. The main structural element of the proposed device is shown in Figure 1(a). This nano-memory device is based on the MWCNT’s telescoping motion relative to each other, which has been extensively investigated [8].

![Figure 1](image-url)

Figure 1. A general design of MWCNT-based nonvolatile memory. (a) The initial equilibrium position, (b) the core CNT contacts with the right electrode with $V_1$ and (c) the core CNT contacts with the right electrode with $V_2$. 
The energetic schematics of the MWCNT memory are shown in figure 2. The total energy of the MWCNT memory is composed of both C-C vdW energy and CNT-metal binding energy. As the CNT-metal binding energy increases, the localized energy well can be achieved, leading to the bi-stable positions of the core CNT. This device can be applied to binary- or triple-digit memory as shown in figures 1 and 2. For binary digit memory, both the ‘state 0’ and the ‘state 1’ are the ‘bit 0’ and the ‘state 2’ is the ‘bit 1’. This device can record the complementary digit: in example, the ‘state 0’ is the ‘bit 0’, ‘state 1’ is the ‘bit +1’, and the ‘state 2’ is the ‘bit –1’. For triple digit memory, the ‘state 0’ is the ‘bit 0’, ‘state 1’ is the ‘bit 1’, and the ‘state 2’ is the ‘bit 2’.

![Energetic schematics of the telescoping MWCNT-based memory.](image)

The logic information at every memory element is determined by measuring the resistance of the junctions [6,8]. The ‘state 0’, of free-of-contact state, refers to a sufficient gap between the core CNT cap and the left or right surface such that there is no conduction pathway between the CNT and the electrodes (figure 1(a)). Conversely, both the ‘state 1 and 2’ refer to the electrical contacts between the left and the right electrodes of the device through the telescoped core CNT and the electrodes of the device through the telescoped core CNT of the MWCNT (figures 1(b)-(c)). It is known that the CNT-metal binding forces provide the electrical contacts of conducting materials, and so a conduction pathway between the telescoped core CNT and the electrodes exists in the turn-on state. The turn-off state conductance must be much lower than the conductance of the turn-on state so, by measuring the resistance at the junction, it is easy to determine the current position of the core CNT, and therefore to distinguish zero from null in the information bit.

The forces acting on the CNT memory is demonstrated in figure 3. The potential differences between the CNT and the electrodes induce capacitive forces ($F_C$). So the movable core CNTs can be extracted from the MWCNT by the capacitive force and can be moved outwards. When the movable CNTs are partially extruded, the suction force ($F_{vdW}$) exerted by the excess vdW energy acts on the movable CNTs and is the same as the restoring force of the MWCNT memory. Therefore, when the applied voltage is above the threshold, the driving force ($F_D$) can make the movable CNTs to escape from the MWCNT and then, the core CNT contacts with the electrode. The state can be divided by the electrode contacted with the CNT, as shown in figures 1(b)-(c). Using both electrodes, the state transition can be achieved when the attractive capacitive forces ($F_C$) are higher than the CNT-electrode binding force ($F_B$). Therefore, the FB should be not high in order to have a low transition voltage. Another force contribution arises from the interwall repulsion force ($F_R$) within the MWCNT because the walls in the MWCNT have the same charge.
Figure 3. An operation principle of MWCNT-based nonvolatile memory. \( F_C \) is capacitive forces, \( F_{vdW} \) the suction force exerted by the excess vdW energy, \( F_B \) the CNT-electrode binding force and \( F_R \) the interwall repulsion force within the MWCNT because the walls in the MWCNT have the same charge.

The capacitive force between the CNT cap and the electrode can be simply modeled by the electrostatic force between a charged plane and a sphere [11]. It is known that the electrostatic force between a charged plane and a sphere can be evaluated analytically by the approximate formula:

\[
F(z) = \pi \varepsilon_0 \frac{R^2}{z(z + R)} V^2
\]

where \( z \) is an instantaneous gap between the plane and the sphere, and \( R \) is a sphere radius, \( V \) is voltage, or electric potential, and \( \varepsilon = 8.854 \times 10^{-12} \text{ Fm}^{-1} \) is the free-space permittivity for air. The interwall repulsive force within the MWCNT was modeled as force between two halves of a charge sphere expressed by the manner proposed in the previous work [9].

3 RESULTS AND DISCUSSION

Figures 4(a)-(b) show the energetics obtained from the static simulations for Pt and Au surfaces, respectively. For each 0.01 \( \text{Å} \) increase of the central position of the inner (5,5) CNT, the structure was optimized by the steepest descent (SD) method and then, the potential energies and the excess forces were calculated. The energetics obtained from the simulations are similar to the schematics of figure 2. Since the CNT-Pt binding energy is higher than the CNT-Au binding energy, the localized potential well depth for the Pt surface is higher than the that for the Au surface, and for the localized states, the excess force on the (5,5) CNT for the Pt surface is higher than the for the Au surface.

For Pt and Au surfaces, the central position variations of the (5,5) CNT are displayed as a function of the applied voltage in figure 5. Each cycle is divided by 8 parts as follows: the \( V_1 \) linearly increases to 6 \( \text{V} \) within 20 \( \text{ps} \), maintains in a constant 6 \( \text{V} \) for a sustaining time, linearly decreases to 0 \( \text{V} \) within next 20 \( \text{ps} \), and has a constant 0 \( \text{V} \) for a sustaining time. This is the half of the cycle. The \( V_2 \) has a constant 0 \( \text{V} \) for the half of the cycle; then, the \( V_2 \) linearly decreased to \( -6 \text{V} \) within 20 \( \text{ps} \), has a constant \( -6 \text{V} \) for a sustaining time, linearly increase to 0 \( \text{V} \) within the next 20 ps, and the \( V_2 \) has a constant 0 \( \text{V} \) for a sustaining time. The sustaining times considered in this work are 20, 30 and 40 \( \text{ps} \).

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For the sustaining time of 20 \( \text{ps} \), the \( z_{CNT} \) is plotted as functions of \( V_1 \) and \( V_2 \) in figure 6(a) and as functions of the MD time in figure 6(b), respectively. \( V_1 \) and \( V_2 \) variations are also plotted in figure 6(b). The controllable CNT position can be explicitly determined. The energetics obtained from the MD simulation of figure 6 are displayed in figures 7(a)-(d), which show the vdW potential energy \( U_{vdw} \), the potential energy between the CNT and the right electrode \( U_{CNT,R} \), the potential energy between the CNT and the left electrode \( U_{CNT,L} \), and the total potential energy \( U_{CNT} \), respectively.
and the left electrode ($U_{CNT-M2}$), and the excess force on the CNT ($F_{CNT}$), respectively. The energetics obtained from the MD simulation show the locally stable states of the CNT shuttle to be applied to a nonvolatile memory. However, as seen in figure 6, the CNT shuttle could not be stabilized on the metal surface because of the short sustaining time of 20 ps. The switching of the CNT memory was achieved form the voltage control, but some of the memory states were not maintained because it was difficult for the CNT to settle on the metal surfaces for the sustaining time of 20 ps.

![Figure 6](image)

Figure 6. (a) $z_{CNT}$ as functions of $V_1$ and $V_2$ and (b) $z_{CNT}$, $V_1$ and $V_2$ as a function of the MD time for Pt electrodes with the sustaining time of 20 ps.

4 SUMMARY

We proposed a novel CNT-based nonvolatile memory serving as the key building block for molecular-scale computers and we performed MD simulations to investigate the dynamic operations of a double-walled CNT memory. The most important physical characteristics of the proposed nano-memory device are the bi-stability governed by the C-C vdW and CNT-metal binding energies and the reversibility led by electrostatic attractive forces. The material for the electrodes could be carefully chosen to achieve the non-volatility of this memory. MD simulations showed that the Pt electrode was better than the Au electrode. The kinetic energy of the CNT shuttle experiences the several rebounds induced by the collisions of the CNT onto the metal electrodes, and this is critically important to the performance of such an electrostatically telescoping CNT memory because the collision time is sufficiently long to cause a delay of the state transition.

REFERENCES

[8] Maslov L 2006 Concept of nonvolatile memory based on multiwall carbon nanotubes Nanotechnology 17 2475