Reversible mechanical bistability of single-walled carbon nanotubes under axial strain

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Using Brenner's second generation reactive empirical bond order potential, we show by molecular dynamics that the single-walled carbon nanotube with a diameter of about 5 nm under axial strain possesses excellent reversible mechanical bistability. This feature provides a high potential of using only one single-walled carbon nanotube to realize bistate functions in nanomechanical systems which will benefit from smaller size significantly. © *2006 American Institute of Physics*.
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Carbon nanotubes (CNTs) have been proposed as one of the most promising materials for nanoelectromechanical systems (NEMS) due to their superior mechanical properties (e.g., high elastic modulus, high failure strength, and excellent resilience), amazing electronic properties (can be either metallic or semiconducting, depending on their chirality), as well as unique coupled electromechanical behaviors (e.g., their conductivities are very sensitive to the deformations).[1] For instance, carbon nanotubes have found applications as many NEMS devices such as nanotweezers,[2] nanoactuators,[3] nanoswitches,[4] nanosensors,[5] and random access memory (RAM) elements.[6–8] Among various applications in these works, one attractive branch is that in which the exceptional mechanical properties (e.g., excellent resilience and high failure strength) of CNTs are used to realize the reversible bistability that is necessary for the definition of on and off states of a CNT-based element in many NEMS. The bistability can arise from the interplay of the elastic energy stored in the nanotube via mechanical deformation and the attractive van der Waals energy resulted from the interaction between the tube and something else, such as another nanotube[2,7] or fullerene,[6] or the substrate.[4] On the other words, there need another object for a nanotube to realize reversible bistate functions, which actually brings much difficulties to the construction of the designed devices.

In this letter, via molecular dynamics calculations, we show that a single-walled carbon nanotube (SWCNT) with a diameter of about 5 nm under axial strain possesses excellent reversible mechanical bistability. This means that one can use *only one* SWCNT without need of the interaction from the substrate or another nanotube or fullerene to realize bistate functions. This feature provides a high potential of SWCNTs in nanomechanical systems.

The molecular dynamics simulations were carried out using Brenner's second generation reactive empirical bond order potential[9] (REBO) to describe the short range bonding energies among carbon atoms. The long range van der Waals interaction is calculated by Lennard-Jones 12-6 potential with well-depth energy of $\varepsilon=4.7483\times10^{-22}$ J and equilibrium distance of $\sigma=0.3407$ nm. The Berendsen thermostat[10] were used to keep the system at the specified temperature (300 K) and a 2 fs time step was used in all molecular dynamics (MD) simulations. A velocity Verlet algorithm[11] was adopted to integrate the equations of motion. The SWCNT was axially loaded by applying a rate of 18 m/s to the last three rings at each end of the tube inwardly. The radial displacements of the atoms on these rings are constrained to result in a clamped condition at the two ends of the SWCNT.

We show in Fig. 1 the morphology changes of an axial strained (55, 0) SWCNT that has 19 910 atoms and is about 38 nm long. The SWCNT was firstly loaded by axial compression. At a critical buckling strain of $\varepsilon_b=-1.01\%$ (here "−" is used to represent a compressive strain), the tube buckled into a diamondlike pattern. The value of the critical strain agrees well with those given by the analytical models,[12–14] validating the accuracy of the present numerical

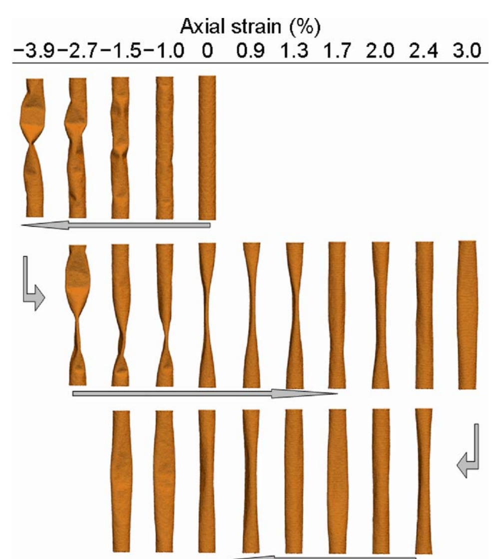

FIG. 1. (Color online) Morphological changes for (55, 0) nanotube under axial strain.

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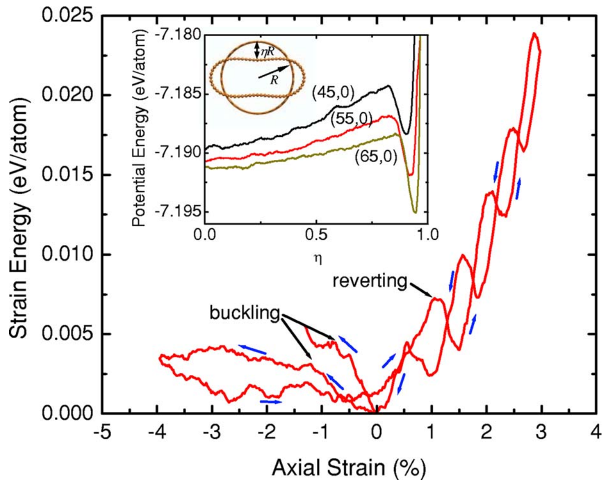

FIG. 2. (Color online) Strain energy for (55, 0) tube vs axial strain. Arrows indicate the loading directions. Inset: potential energy against flatness of radial compressed nanotubes.

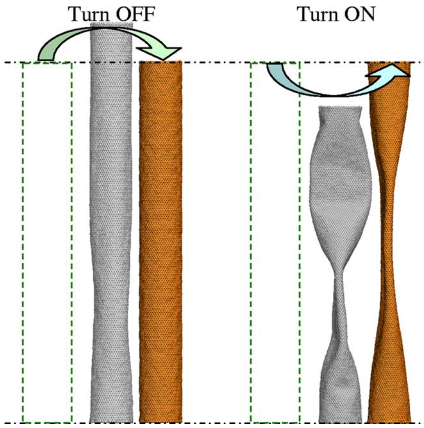

FIG. 3. (Color online) Schematic illustration of SWCNT based nanoswitch. The switch can be turned off by stretching then releasing the tube, and turned on by compressing then releasing it.

simulations. With a further increasing of the axial compressive strain, the SWCNT collapsed into a piecewise ribbonlike structure (or in the extreme, the main body of the SWCNT is ribbonlike except that the two ends are still kept cylindrical shape due to the clamped constraint). The unloading process for axial compression started at about $\varepsilon=-4\%$. What we should pay special attention to is that the SWCNT retains collapsed structure when the axial strain was reduced to less than the critical buckling strain. Even the axial compressive strain was totally removed, the (50, 0) SWCNT still kept its collapsed ribbonlike structure. An axial tension strain was then applied to the SWCNT in the further calculation. It is found that the SWCNT would revert its cylindrical structure at $\varepsilon_r=1.29\%$ (we name it the *critical reverting strain* for convenience). The axial tension strain is further increased to about 3% in our calculation. We note that reverting may cause a second order radial vibration of the tube wall. Although the tube sometimes looks very like in a ribbonlike shape at this stage, it does not mean that the tube is in collapsed structure because the minimum spacing between its opposite walls is much larger than that in a collapsed tube (i.e., ~0.34 nm), and the radial vibration would eventually damp out and the tube would be left as a cylindrical shape. The axial tension strain was then released and the compressive strain was added again. It is found that the SWCNT retains its cylindrical structure until the compressive strain approaches the critical buckling strain (note that the critical buckling strain this round is somewhat less than the first round due to the presence of the radial vibration which actually weakened the axial stability of the tube). No irreversible (plastic) deformation is found in the above loading process. This indicates that the (50, 0) SWCNT under an axial strain in the interval of $(\varepsilon_b, \varepsilon_r)$ possesses reversible bistability. In particular, the (55, 0) SWCNT at zero axial strain could maintain both the cylindrical and collapsed structures. More importantly, the two stable states of the SWCNT can be switched from one to the other by the applied axial strain, which provides a high potential of carbon nanotubes in nanomechanical devices, as will be discussed below.

The mechanical bistability of a SWCNT arises from the interplay of the elastic energy, which is stored in the nanotube via mechanical deformation, and the attractive van der Waals energy, which is resulted from the interactions between atoms on collapsed region. The elastic energy of a SWCNT tends to maintain the tube as a cylinder, while the van der Waals energy may provide attractive force to attempt to keep the tube as a ribbonlike structure once it collapsed. Hence, the bistability appears only for the SWCNT with moderate diameters (say about 2–6 nm) in which the two competitive energies are comparable. For relatively small or large SWCNT, one of the two competitive energies (elastic or van der Waals) plays a dominant role, and the other is relatively ignorable, leading to the vanishing of the bistability. An earlier study by Gao *et al.*[15] on the structure stability of freestanding SWCNTs showed similar results. They observed the structural optimization of SWCNTs with two kinds of initial structures: (1) perfect circular cross section and (2) collapsed cross section. Only the tubes with radius between the two transition radii R_1(≈1 nm) and R_2(≈3 nm) have bistable form. Similar phenomenon has been experimentally observed by Chopra *et al.*[16] more earlier for multiwalled carbon nanotubes. Using a simple analytical model presented in that work, a SWCNT with a radius of about 3 nm possesses the best bistability, which are in reasonable agreement with the current calculations.

Strain energy (simply averaged over tube volume and adjacent 50 time steps) of the (55, 0) nanotube corresponding to the axial strain is shown in Fig. 2. It is shown that about 3 meV/atom is required to change the tube from cylindrical state to collapsed state, while 7 meV/atom is required for the reverse process. To give a clearer understanding of the bistability of SWCNTs, we performed molecular dynamics simulations for radial compressed (45, 0), (55, 0), and (65, 0) tubes with lengths about 2.5 nm. The potential energy versus the tube flatness is shown in inset of Fig. 2. We can see that the collapsed structure of (55, 0) tube is the stable state, while the cylindrical shape is the metastable one.

Many studies have shown that mechanical deformation will dramatically influence the electrical conductance of a SWCNT.[17–19] For instance, the resistance of a semiconductor SWCNT in cylindrical shape will be very high, while its resistance in ribbonlike or buckling structure will be orders of magnitude lower. Considering the above observed reversible mechanical bistability, we can design a SWCNT-based nanoswitch using only one semiconductor SWCNT whose cylindrical and ribbonlike structures provide, respectively, well-defined off and on states. The switch can be turned on

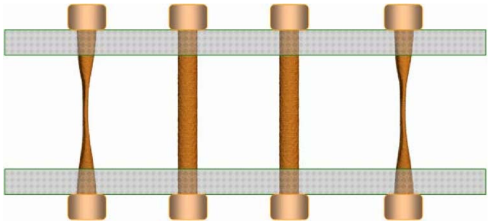

FIG. 4. (Color online) Schematic illustration of SWCNT based random access memory with two elements in the on state (collapsed) and two elements in the off state (cylindrical). The two ends of each element are connected with electrodes which are used to electrically check the information stored in the element. The main body of each element is constrained by two parallel electrically isolating substrates.

by compressing then releasing the tube, and turned off by stretching then releasing it (see Fig. 3).

The nanoswitch can serve as a RAM element. The structure of the RAM is shown in Fig. 4. The RAM device consists of a larger number of highly ordered parallel SWCNTs whose two ends are connected with electrodes and whose main bodies are constrained by two parallel electrically isolating substrates. The element can be switched by axial strain, and the information stored in it can be read by measuring its conductance. The most advantage of such a RAM device lies in two aspects. First, it would take up much less space and thus provide much higher access density (up to $\sim 100\ \mathrm{T/cm^2}$) because only one SWCNT is used as an element. Second, the self-assemble techniques on the SWCNT array[20] can be adopt to produce the RAM structure in large scale and there is no need of the direct manipulation of nanotubes in constructing a RAM. In addition, the RAM provides many other useful features such as nonvolatility, high responding rate ($\sim$100 ps), low energy consumption, long life, and so on. An experimental study on this subject by the authors' group is in progress.

Besides the electrical applications, the switch we presented above can also be used to control fluid flow. In this case, however, the on and off states are reversed. Namely, the switch is on if the SWCNT is in cylindrical shape, while when the SWCNT is collapsed, the switch is off because the fluid flow through the tube is forbidden, unless a critical inner pressure is approached to open the switch.

In summary, we show by molecular dynamics simulations that a SWCNT with moderate diameter under axial strain possesses reversible mechanical bistability, which provides a high potential of SWCNTs in nanomechanical devices. Some possible applications have been outlined in the letter.

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