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Theoretical Study of SET Operation in Nantero Memory Cell

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We present results of self-consistent electronic structure calculations for an electromechanical memory cell consisting of a carbon nanotube (cnt) fabric between titanium leads to elucidate the mechanism whereby the applied bias works to close the current gaps in the cnt fabric. We demonstrate that the asymmetry in the bias conditions required to achieve the "SET" operation of the cell (changing it from a high resistivity to low resistivity) results from the nature of a voltage drop in a compensated semiconducting material and depends sensitively on the background charge as well as on the position of the layer where the conducting gaps occur. The calculations provide insight into the behavior of the material and suggest possible fabrication strategies to modify the functionality.

A cross section of the memory cell is shown in figure 1, (a) the 2D layers, (b) the individual cells after patterning, along with (c) a schematic of the calculation. The device consists of layers of spun cnts deposited on a TiN bottom contact and covered by a deposited TiN top contact. The contact to contact distance (the thickness of the cnt layer) can be varied but is typically 20-40 nm. The 2D area of each cell (also variable) is on the order of $1\mu m^2$. The simulation, as opposed to the actual device, is two dimensional, thus there is only one direction (y) perpendicular to the line between the contacts (x). All the nanotubes (blue circles) are assumed to lie perpendicular to the plane of the paper. Thus the simulated device consists of a set of nanotubes that are infinite in the third direction.

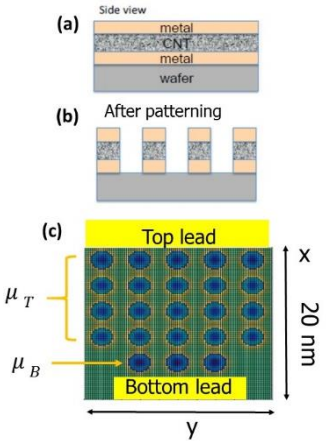

Figure 1: schematic of (a) 2D layer structure, (b) patterned cells and (c) simulation geometry. See text.

While the electrostatics (i.e. Poisson's equation) is 2D, the filling of states assumes both 2D wave functions in the x-y plane and a density related to the cnt density of states. The charge density is given by

$$\rho(x,y) = \sum_{n,m} \left|\Psi_{n,m}(x,y)\right|^2 \int \frac{dk}{2\pi} f\left(\varepsilon_{n,m}(k) - \mu_m\right) \quad (1)$$

where $\Psi_{n,m}(x,y)$ is the transverse wavefunction for the nth state of the mth nanotube, $\varepsilon_{n,m}(k) = J_n\, cos(ka) + E_n^0 + V_{nm}$ is the state energy which we take as a tight binding form with parametric n-bandwidth J_n, bare energy E_n^0, and Coulomb energy (matrix element of the state with the electrostatic potential) V_{nm}, and f is the Fermi function. Note that V_{nm} depends on m, the cnt index, and accounts for the self-consistent interaction with the potential at the position of the mth cnt. Note also that the chemical potential μ_m depends on the nanotube. We set this chemical potential to the chemical potential of the bottom lead for some of the tubes and to that of the top lead for the others (we ignore the metal ionization potential for simplicity). In the example shown in figure 1(c) the bottom row of cnts is fixed to μ_B and the others are fixed to μ_T. In a self-consistent calculation, this chemical potential difference leads to a voltage drop between the layers with the differing potentials (see results below).

Variable parameters include the sizes, number and positions of the nanotubes, lead voltages, $V_{T,B}$, and a background charge density ρ_+ which is taken as static (i.e. the ionization state of all donors or acceptors is assumed to be fixed). This background charge is placed in circular disk regions centered on and of the same diameter as the cnts. Figure 1(c) shows the total charge density and the center (blue) regions of the cnts are dominated by the background charge.

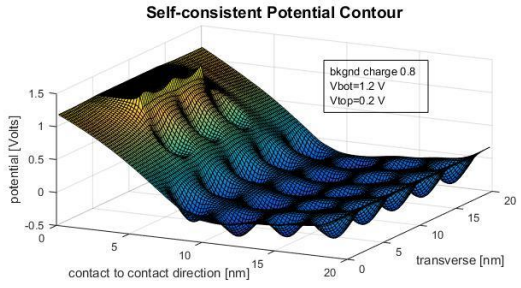

Figure 2 Potential contour from bottom (left) to top. First row of three cnts pinned to bottom chemical potential. Remaining cnts at top potential. Force to close gap proportional to voltage drop from rows 1 to 2.

A typical result for the self-consistent potential is shown in figure 2. Here, $V_B = 1.2\,V$ and $V_T = 0.2\,V$. The background charge is set to 80% of the total electric charge. As in the figure 1(c) example, the bottom three cnts are filled to μ_B and the others to μ_T. Note therefore that the potential drops the greatest between layers 1 and 2. In the "RESET" (high resistance) state of the device, a gap is assumed to exists in the cnt material between certain layers. In this example the gap is between layers (cnt rows) 1 and 2. The potential drop between those layers is thus proportional to the force acting to close that gap.

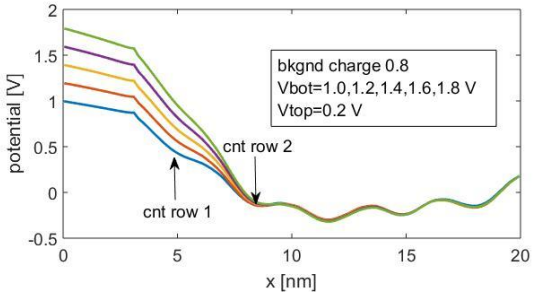

Figure 3 Potential drop along lead to lead (x) direction averaged over y for several bottom voltages. Vtop=0.2 V.

It is useful to average the potential along the transverse (y) direction (Fig. 3) and plot the potential drop versus applied voltage. Here the top is held at 0.2 V and the bottom is varied from 1.0 to 1.8. Clearly increased voltage increases closing force. When the polarity is reversed, (Vtop sweep) the drop appears as in Fig. 4. In the inset to Fig. 4, the row 1 to 2 voltage drop is plotted versus the applied voltage. Clearly the bottom lead is more effective at creating a voltage drop between the two rows. Therefore an asymmetry in the required voltage to "SET" the memory cell is observed, consistent with experiment.

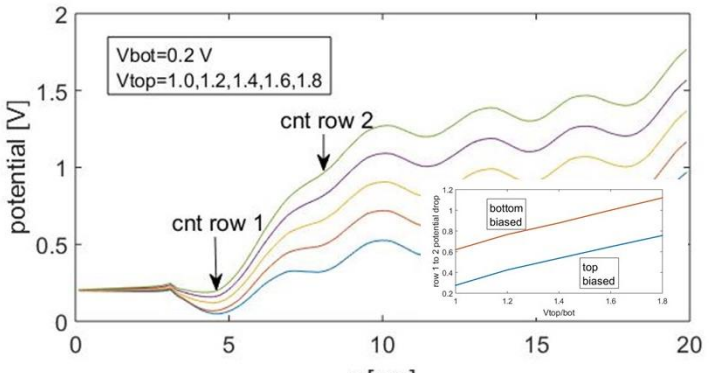

Figure 4 Same as Fig. 2 but top lead varies. Inset: bottom lead is more efficient at creating voltage drop from 1 to 1.

There are two manifestations of device asymmetry in the simulation: (1) the location of the gap (closer to the bottom) and (2) the size of the leads (the bottom lead is smaller). It is the gap location which is crucial in determining the asymmetry of the SET operation. This results from voltage dropping between the top lead and the 1 to 2 gap (i.e. between top and row 2). This voltage drop is sensitive to the background charge and the asymmetry is seen to vanish as the background charge vanishes (and the device becomes "intrinsic"). Further results and analysis will be given at the talk.