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Calculation of the Electromechanical Properties of CNTs Under Deformation by Means of a Novel Numerical Model

The effects of mechanical deformation on the electron transport behavior of carbon nanotubes (CNTs) are of primary interest due to the enormous potential of nanotubes in making electronic devices and nanoelectromechanical systems (NEMS). Moreover it could help to evaluate the presence of defects or to assess the type of CNTs that were produced. Conventional atomistic simulations have a high computational expense that limits the size of the CNTs that can be studied with this technique. Here we present a novel numerical approach able to simulate the electromechanical behavior of SWNTs and MWNTs of the dimensions used in nano-electronic devices. The numerical model was designed to realize orders-of-magnitude savings in terms of computational time in the calculation of the mechanical behavior and of the changes induced by the deformation in the electrical transport properties of the nanotubes. The computational method has been validated with respect to fully atomistic simulations and to a simulation of laboratory experiments. In this paper, simulation results are presented for different types of SWCNT and MWCT in a variety of boundary conditions.

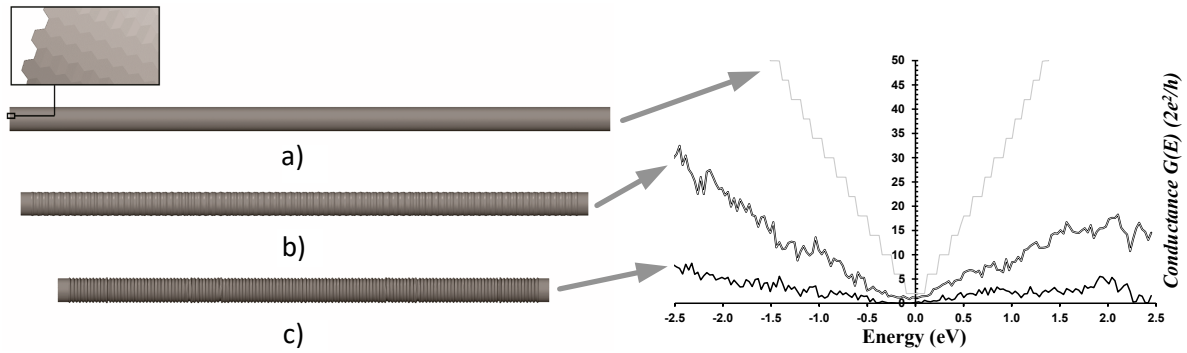

Figure 1: Model reproducing a MWCNT: a) in the undeformed configuration, b) compressed axially by 20 nm, c) compressed axially by 50 nm. The inset shows a magnification of the outermost wall revealing the hexagonal cells.

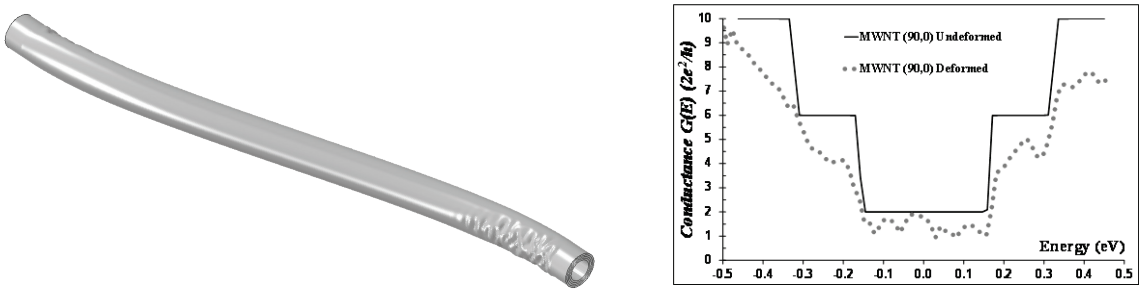

Figure 2: Simulations of a MWCNT where the two ends of the tube have been misaligned by 30 nm.

References

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