Simulation of Nanotube Devices

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The **device modeling** has been performed for several Nanotube Electromechanical Systems (NEMS) and nanotube capacitors. A **compact model** has been developed for the calculation of such device parameters as nanotube deflection and shape, voltage drop, charge distribution, distributed capacitance and depolarization. The model was successfully applied to the nanotube actuator, the nanotweezers, and the nanoswitch (shown in Figure) [1,2,3]. The model includes elements of quantum mechanical consideration through the calculation of the nanotube polarizability, atomistic capacitance [4,5], and van der Waals interaction [6].

The physics of carbon tubes is rather distinct from the physics of standard semiconductor devices and it is unlike that device modeling can be simply transferred to the new case. Several issues, including the van der Waals interaction, the shell crystal structure, elasticity theory for shells, the strictly one-dimensional electronic structure and one-dimensional electrostatics, are to be solved.

Main advantage of our modeling is the use of **continuum approach** for the nanoscale system. Numerous Molecular Dynamics simulations and analytical calculations done to date confirmed this continuum approach. Extensive data validates the use of (1) the continuum description of the electronic structure and selfconsistent electrostatics, (2) the continuum description of the deformation/deflection of NEMS, (3) the continuum description of the van der Waals energy.

The discussed results are:

- the calculation of main parameters for nanotube actuator device [1,3], such as: pull-in voltage, critical deflection;
- the atomistic theory for the one-dimensional device electrostatics [4,5]: nanotube capacitance as depending on the device design, nanotube symmetry and nanotube shape (deformations);
- the analytical theory of NEMS operation [3,6], which reveals the van der Waals and other atomistic contributions to the device equation-of-state; analytical expressions for main device parameters allows one to do fast and precise estimations for various geometry and design.

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Figure

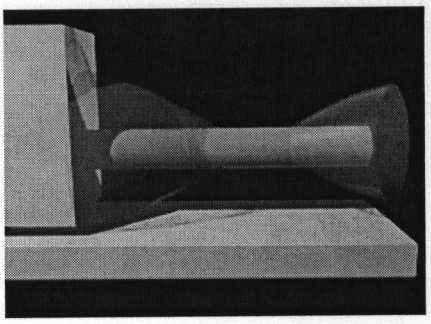

Figure. Design of typical Nanotube Electromechanical system. The tube is connected to a side electrode and suspended over a back-gate.