Atomistic Models for Nanotube Device Electrostatics

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The 1D character of the electromagnetic eigenmodes of SWNT system results in a weak screening of the Coulomb interaction and the external field. Below we present a quantum mechanical calculation of the polarizability of the metallic [10,10] tube. This quantity is not defined solely by the intrinsic tube properties. In contrast, it depends also on the geometry of the nanotube, and/or the closest gates/contacts. Hence, the charge distribution has to be considered selfconsistently. The local perturbations of the electronic density will influence the entire system unlike in common semiconductor structures.

Figure 1 is a sketch of the depolarization of the tube potential (induced charge density) by the side electrode and the back-gate. The green continuos line is the statistical approximation (Boltzmann-Poisson eqs.) which coincides well with the Quantum Mechanical result (blue dotted line) except for the quantum beating oscillations at the tube end. The depolarization manifests as a significant nonuniformity of the charge along the tube length.

In one-dimensional systems, the potential, ϕ^{act}, induced by a charge density, ρ^{ind}, is proportional to this charge density. Thus, the Poisson equation is effectively reduced to

$$\rho^{\mathrm{ind}}(z) = -e^2 \nu_M \phi^{\mathrm{act}}(z).$$

Here ν_M stands for the nanotube density of states. We demonstrated that this quantity works as an atomistic capacitance of a SWNT:

$$C_A^{-1} = \frac{1}{e^2 \nu_M}$$

and

$$C_m^{-1} = 2 \log\left(\frac{2h}{R}\right)$$

gives the geometric capacitance which is a function of distance to the back-gate and SWNT radius, in case of straight SWNT it is a logarithm. In equilibrium, we write a relation between the equilibrium charge density and external potential (gate voltage), which comprise both the atomistic and geometric capacitance:

$$\rho_\infty = -\frac{\varphi^{\mathrm{xt}}}{C_m^{-1} + C_A^{-1}} \simeq$$
$$\simeq -\varphi^{\mathrm{xt}}\, C_m \left(1 - \frac{C_m}{C_A}\right)$$

The last equation is still valid for the nanotube of an arbitrary shape, although, no simple expression for the geometric capacitance C_m can be written for a nanotube when it is bent.

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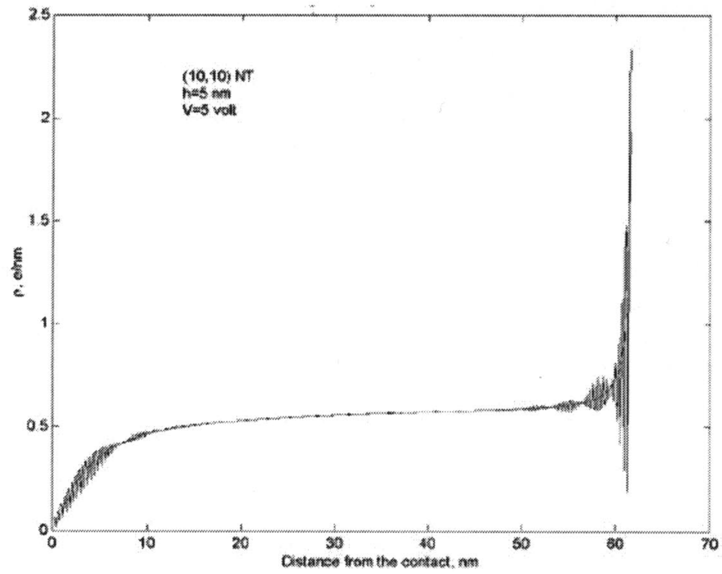

Figure 1. Selfconsistent charge density of a [10,10] armchair nanotube at 5 V voltage applied between side and back-gate contacts. The distance between the tube center and the back-gate is 5 nm, the tube radius and length are 0.6 nm and 60 nm.