Quantum transport simulation of a graphene field effect transistor

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BACKGROUND

We have implemented a self-consistent tight-binding model for modeling transport in nano-scale devices[1,2]. The basic electronic structure of the device is obtained with a self-consistent Slater-Koster or extended Huckel tight-binding model which can be fitted to experimental or accurate theoretical reference data. The charge in the device is calculated using non-equilibrium Green's functions (NEGF), and the corresponding electrostatic potential is obtained by solving the Poisson equation. The model allows for fast and accurate transport calculations of large nano-scale devices.

MODELLING A GRAPHENE TRANSISTOR

We will calculate the electrical properties of a 34 Å and 86 Å long graphene nano transistor, illustrated Fig. 1. The system has two metallic electrodes made of zigzag-edge graphene nano-ribbons. The electrodes are connected through a semi-conducting armchair-edge central ribbon. The system is placed 1.4 Å above a dielectric material with dielectric constant 4, corresponding to SiO_2. The dielectric is 3 Å thick, and below the dielectric there is an electrostatic gate.

TRANSISTOR CHARACTERISTICS

Figure 2 shows the current for an applied source-drain voltage of 0.2 V as a function of the applied gate potential, for gate potentials in the range −1 to 1 V, and at 150, 300, 450 K electrode temperatures. The short device shows only a small effect of the gate potential and electron temperature while the conductance of the long device falls off exponentially, reaching a minimum in the range 0–0.5 V. Moreover, the current is strongly temperature dependent.

The lack of temperature dependence for the short device shows that the transport is dominated by electron tunneling. The strong temperature dependence of the long device shows that in this case the electron transport is dominated by thermionic emission. The dotted lines illustrate the $1/kBT$ slope expected for thermionic emission, and in the gate voltage range from −0.25 to −0.75 V, the *I-V* characteristics follow these slopes well.

Figure 3 shows the electrostatic profile through the device. Note how the gate potential is almost perfectly screened by the graphene layer. This means that for a layered structure, only the first layer will be strongly affected by the backgate. This has implications also for gated nanotube devices. In such a device, only the atoms facing the gate electrode are strongly influenced, and this explains why in Ref. 3 we found that the transport in the device was dominated by tunneling even though the nanotube was 110 Å long, and thus longer than the graphene junctions studied in this paper. This illustrates that efficient gating of a nanotube, can only be obtained if the gate electrode wrap around the tube.

CONCLUSION

In this paper we have introduced a semiempirical model for electron transport in nanodevices. The model was used to model a graphene nano transistor, and our study illustrates how the transport mechanism changes from tunneling to thermionic emission as the device is made longer.

REFERENCES

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[2] Calculations have been performed with Atomistix ToolKit (ATK 10.8), www.quantumwise.com.
[3] H. H. B. Sørensen, P. C. Hansen, D. E. Petersen, S. Skelboe, and K. Stokbro, *Efficient wave function matching approach for quantum transport calculations*, Phys. Rev. B **79**, 205322 (2009)

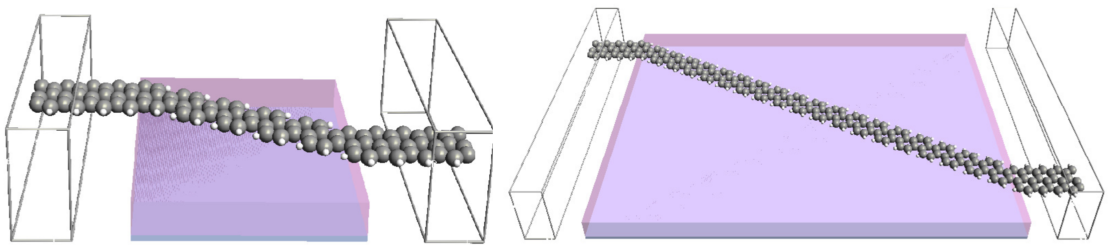

Fig. 1. Geometry of the 34 Å and 86 Å long graphene field effect transistor studied in this paper.

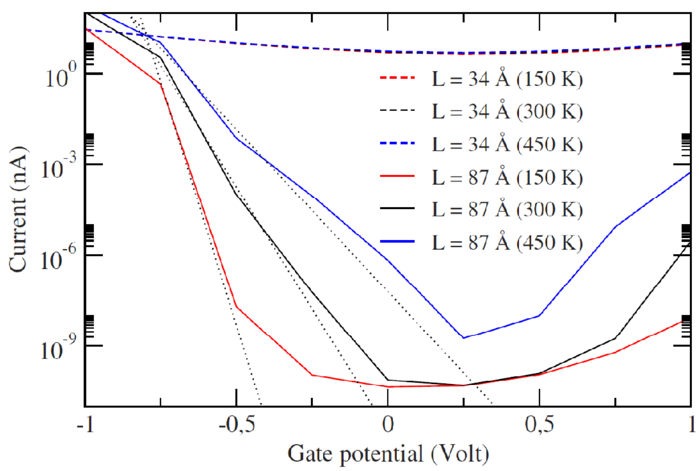

Fig.2 Current as function of gate potential for a source-drain bias of 0.2 V. Different curves are for different electron temperature in the electrodes. The current for the 87 Å device follows a $1/k_bT$ slope (dashed lines) and the transport is dominated by thermionic emission. The current in the 34 Å device has a negligible temperature effect, and the transport is dominated by tunneling.

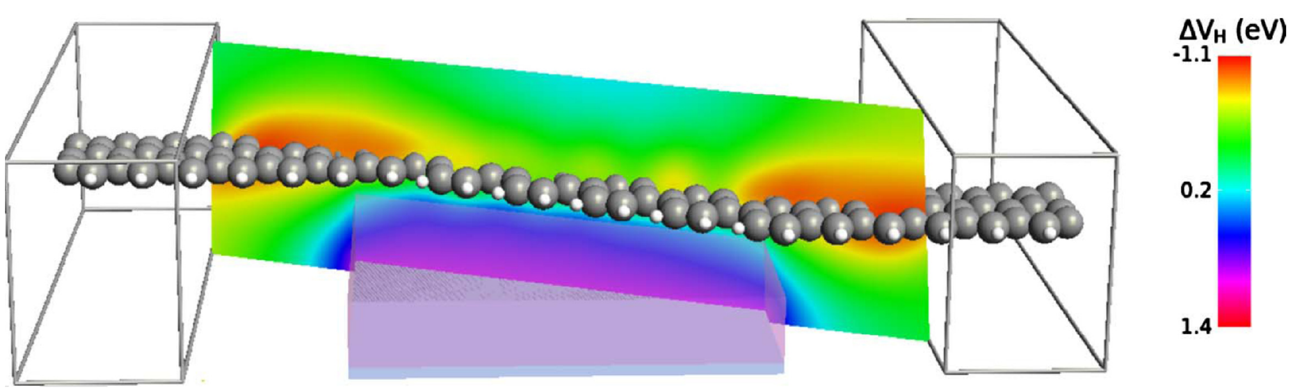

Fig.3. The self-consistent electrostatic potential for a gate potential of -1 V. Note how the electrostatic potential from the gate is screened by the graphene device.