Contacting graphene: First principles transport simulations

Mads Brandbyge[1]

1 Dept. of Micro and Nanotechnology, Center for Nanostructured Graphene (CNG), Technical Univ. of Denmark, build. 345C, DK-2800 Kgs. Lyngby, Denmark

Mads.brandbyge@nanotech.dtu.dk

Devices based on stacked van der Waals heterostructures of two-dimensional (2D) materials are promising candidates for future atomically thin, flexible electronics. Graphene can play the important role of a 2D electrode material due to its excellent semi-metallic electronic conduction. However, we still need to understand and control the behavior of the graphene electrodes for contacting other 2D materials. The same is the case for the metal-graphene contacts used to contact graphene in the first place.

A key advantage of graphene electrodes is the precise control of the carrier density by external gates. Atomistic first principles transport calculations, which can take voltage biases, currents, and gate potentials into account, can yield important insights into the behavior of devices. I will in the talk illustrate this point by presenting examples of transport calculations based on Density Functional Theory combined with non-equilibrium Green's functions (DFT-NEGF) [1], or the Boltzmann equation [2].

The examples include the role of the gate and stacking order for the contact resistance between graphene and MoS_2 (see Fig. 1)[3], a gate-induced flexural electron-phonon scattering mechanism in graphene[4], how phonon-scattering in point-contacts to graphene can reveal the electronic coupling between graphene and substrate[5], and finally, the dependence of contact resistance on the metal used for contacting graphene at the edge [6]

References

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Figures

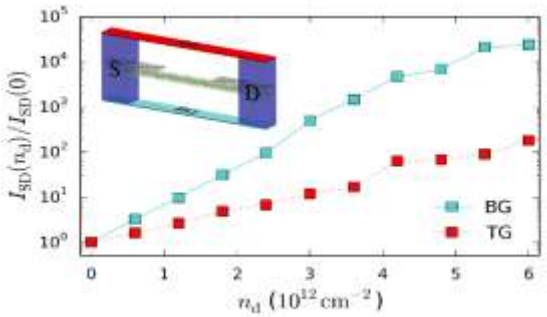

Figure 1. Calculated source-drain current as a function of gate-induced carriers in a graphene-contacted MoS2 channel for gate at top or bottom (insert). From Ref. [3].

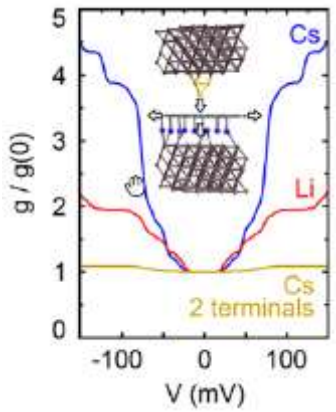

Figure 2. Calculated conductance (normalized to zero bias) as a function of voltage in a STM setup (insert). The sample is Cs or Li intercalated graphene on Ir(111). The sharp increase probes the inelastic phonon signals and reveal the electronic coupling between graphene and substrate. From Ref. [5].