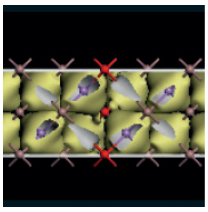

Simulation of contact resistance in patterned graphene

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While trying to exploit graphene in Radio Frequency applications, the reduction of the contact resistance (R_c) is probably one of the most challenging technological issues to be solved. Graphene patterning under the metal has been demonstrated to be a promising solution, leading to a reduction of R_c by up to a factor of 20 [1], probably due to an increased conductivity at the borders of the patterns of graphene [2]–[5]. This technology is still at the early stage and a complete understanding of the physical mechanisms at play is lacking. To this purpose we propose a multi- scale approach based on first-principle calculations, and the solution of the continuity equation to compute R_c in the considered patterned contacts.

The continuity equation in the graphene flake reads:

$$\nabla \cdot J_{2D}(y,z) = |J_{inj}(y,z)| \quad (1)$$

where J_{2D} is a in-plane current density (in A/m), and J_{inj} is the metal-to-graphene vertically injected current, (in A/m^2). In particular, $J_{2D} = \mu\rho\nabla\varphi + D\nabla\rho$, where μ, ρ, D, are the mobility, density, and diffusivity of carriers (either n or p depending on the metal exploited for the contact [6]) and φ is the electrostatic potential. Assuming quasi-equilibrium conditions and neglecting the diffusive term, J_{2D} reduces to $J_{2D} \cong q\mu p\nabla\varphi$. To model the vertical injected current from the overlapping metal, we assume an ohmic relationship i.e., $J_{inj} = G\varphi$ where G is a conductance per unit sur- face (in S/m^2) estimated from atomistic simulations. As a consequence Eq. (1) eventually reads:

$$\nabla q\mu nn\nabla\varphi(y,z) = G\varphi(y,z) \quad (2)$$

Regarding the geometrical structure, we assume that the metal fills the graphene etched regions as in Fig. 1a. The metal-filled regions behave as equi-potential surfaces and can be modeled as Dirichlet conditions for the solution of the differential equation. For what concerns the graphene under the metal, we have considered two different sets of parameters (ρ, μ, G) depending if it is close to the edges of the pattern or far away. An estimation can be obtained from Density Functional Theory (DFT) calculations. Once φ is obtained, we can determine the component along the transport direction (y-direction) of the current density $J2D,y = q\mu nn\,\partial\varphi$ and Rc calculated (in Ω) as:

$$R_c = V_{m-g} / \int dz\, J_{2d,y}(y,z)|_{y=ymax} \quad (3)$$

where V_{m-g} is the metal-graphene bias and the in- tegral accounts for the total current flowing at the contact end, i.e., $_{y=ymax}$.

In this work, inspired by recent experimental results [12], we have considered gold-graphene contacts with graphene patterned with square holes . Two hole sizes (with hole side l_h = 100 nm and l_h = 200 nm) and two different number of holes (n_h = 400 and n_h = 160) have been considered. The graphene region dimension has been set to 12 μm × 5 μm. We have performed DFT calculations using the Quantum Espresso package [7], with a gradient-corrected ex- change correlation functional (Perdew-Burke- Ernzer- hof (PBE)) [8], and a ultrasoft pseudopotentials (US- PPs) [9] in scalar relativistic form. The simulated Au-graphene structure is depicted in Figure 1a. It consists of four continuous layers of Au and an interrupted layer of graphene. Dipole correction and the dispersion effects (Van der Waals corrections [10]) have been included in the simulations. The curve corresponding to the Dirac point energy on graphene in the interacting system has been extracted computing the difference of the local Fermi energies with respect to the vacuum levels and the local work function. The calculated $\Delta Ef = E_d - Ef$ (where E_f is the Fermi level and E_d is the Dirac point) is:

0.32 eV and 0.25 eV, at the edges and the surface graphene respectively (Fig. 1b), resulting in electron concentrations of 7.68 $\times 10^{12}$ cm^{-2} and 4.75 $\times 10^{12}$ cm^{-2}. The electron mobility has been taken equal to 3.5 $\times 10^{3}$ cm^{2}/Vs as in [5]. The geometry of graphene and gold has been optimized keeping the upper two gold layers fixed and relaxing the position of the atoms. Au-graphene equilibrium distances are 3.1 A˚ at the center and 1.9

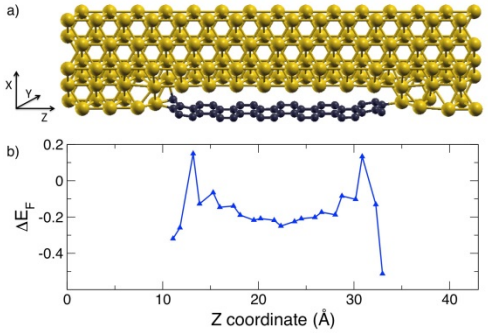

Fig. 1. (a) DFT Au-graphene structure and (b) Fermi energy shift with respect to the Dirac point (ΔE_f) obtained from the electrostatic potential analysis on carbon atoms.

A˚ at the edges. A tight-binding model of graphene has then been used to obtain the transmission coefficient. An electronic gap simulating the gold-graphene interlayer has been introduced by modifying the on- site energies of the graphene Hamiltonian. Using T and ΔE_f we have determined the conductance from Landauer's formalism: $G = \frac{q2}{2\hbar}\int dE \frac{\partial f}{\partial E} T T$ at the edges and the surface respectively. Eq. (2) has then been solved using NanoTCAD ViDES open-source code [11]. We imposed zero potential (as a reference) at the $y = 5$ µm end and set $V_{m\text{-}g}$ = 0.1 V (note that R_c is not dependent on this value). The solution of Eq. (2) for the four different considered configurations is depicted in Fig. 2a. In Fig. 2b we show R_c as a function of the total edge perimeter. As can be seen, as the patterning is increased R_c is reduced in accordance with experimental results. The contact resistance is nonetheless dependent also on the remaining graphene surface, and a large increase of the etched regions spoils the contact [5].

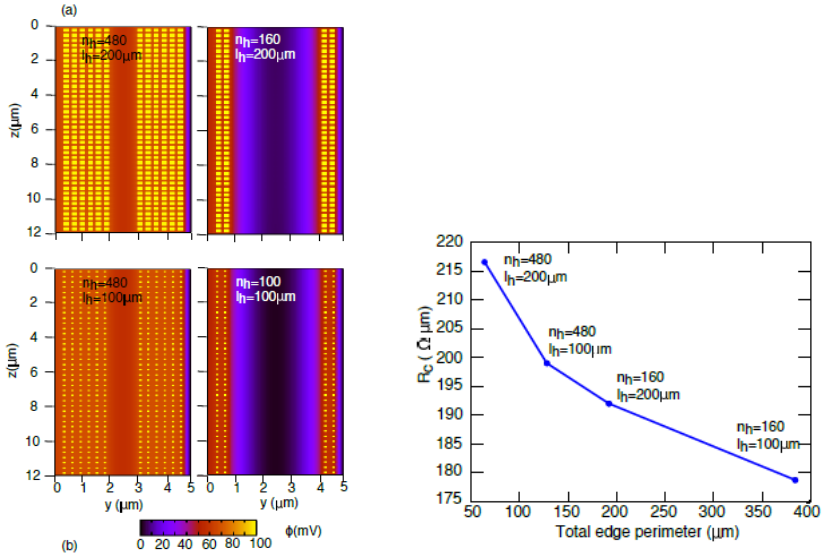

Fig. 2. (a) Potential distribution in the graphene flakes for hole sizes l_h = 200 nm (top) and l_h = 100 nm (bottom) and two number of holes: n_h = 480 (left), n_h = 160 (right). (b) Contact resistance as a function of the total edge perimeter.

A multi-scale approach based on DFT calculations and transport simulations has been proposed to calculate the resistance of metal/patterned graphene contacts. The model has been applied to several pattern configurations and manages to take into account the effects of the edges in reducing R_c. Such a model can be exploited to provide an optimization of the contact resistance and to guide and orient the experimental activity.

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