Graphene nanoislands on Ni(111): structural and scattering properties

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The scattering of electrons at the interface between graphene and metal contacts determines the charge and spin injection efficiency into graphene and, consequently, it is a fundamental issue for the performance of graphene-based devices. Weakly interacting metal contacts simply dope the Dirac bands. The interface with more reactive metals, however, is usually characterized by significant electronic reconstruction, which defines a complex scenario for scattering. The graphene-Ni interface represents an interesting case where the interaction with the ferromagnetic substrate opens hybridization gaps and induces magnetic moments.[1,2] Consequently, graphene is predicted to behave as a perfect spin filter in contact with a magnetic Ni electrode.

In this talk, I will report on the results of a recent combined theoretical and experimental study of graphene nanoislands on Ni(111). Using pin-polarized density functional (DFT) calculations combined with scanning tunneling microscopy (STM) and spectroscopy (STS) measurements, we have studied the structural and electronic properties of this system. We show that the substrate induces the stabilization and reconstruction of the zigzag edges, being the edge structure strongly dependent on the registry of the edge C atoms with the Ni atoms underneath. These results allow us to understand the experimental observation of nanoislands with either triangular or hexagonal shape.[3] Moreover, we find that the electron scattering at the graphene edges depends on the electron spin, on the atomic structure of the edges, and on the orbital character and energy of the surface states.[4] This behavior is attributed to the strong distortion of the electronic structure at the interface, which opens a gap and spin-polarizes the Dirac bands of graphene. This suggests a lateral 2D spin filtering for graphene layers, similar to that occurring across the interface.

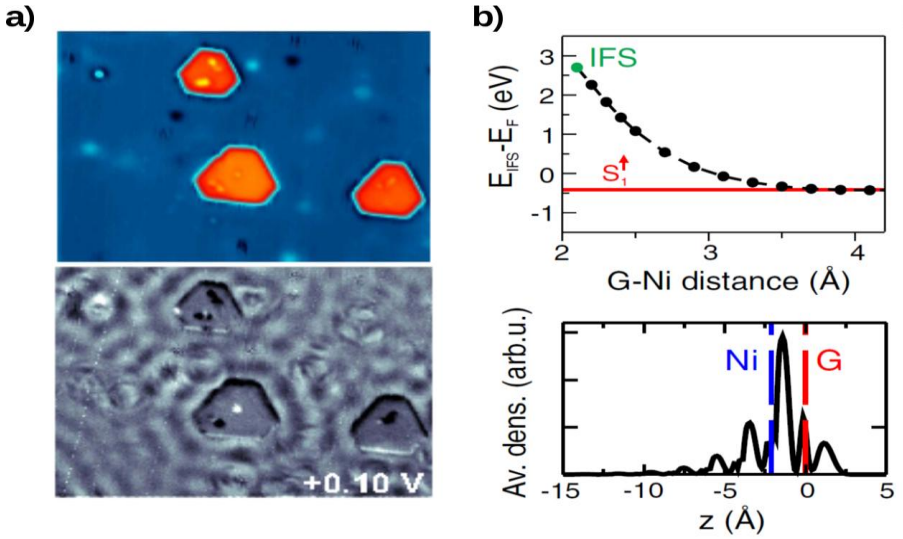

Figure: (a) Topographic (V_b = 0.1V) and constant current dI/dV map showing the interference pattern of the S_1 surface state scattered from graphene islands. Setpoint current: I = 0:3 nA. Image size: 30 x 37 nm^2. (b) Top: calculated energy of the majority interface states (IFS) as a function of the distance between the graphene layer and the Ni surface. The energy of the S_1 surface state for pristine Ni(111) is represented by the red line. Bottom: electron density associated with the majority IFS averaged over a plane at the equilibrium distance (2.1Å).

References

[1] V.M. Karpan et al., Phys. Rev. Lett. 99, 176602 (2007)
[2] M. Weser et al., Appl. Phys. Lett. 96, 012504 (2010)
[3] M. Olle et al., (submitted)
[4] A. Garcia-Lekue et al., Phys. Rev. Lett. 112, 066802 (2014)