Graphene on Ni(100): coexistence of different moiré patterns at a symmetry-mismatched interface

Virginia Carnevali[1,2]
Z. Zhiyu[3], M. Jugovac[1,#], L. Patera[1,§], G. Soldano[4], M. Mariscal[4], C. Africh[4], G. Comelli[1], M. Peressi[1]

[1] *Università di Trieste, Via A. Valerio 2, Trieste, Italy*
[2] *CNR-IOM TASC, Trieste*
[3] *ICTP, Trieste*
[4] *Universidad Nacional de Cordoba, and INFIQC CONICET-UNC, Argentina*
[#] *present address:* Peter Grünberg Institut, Forschungszentrum Jülich, Deutschland
[§] *present address:* Faculty of Physics, University of Regensburg, Deutschland

cavirgi@gmail.com

Epitaxial graphene on metallic surfaces can form a variety of moiré superstructures due to interfacial lattice parameter and/or symmetry mismatch [1] [2]. The latter characterizes graphene on Ni(100), where the hexagonal carbon network accommodates onto a square surface lattice. The interfacial mismatch leads to moiré patterns with stripe-like or rhombic-network morphology and with periodicity depending on the relative misorientation angle between graphene and the Ni surface. Different moiré patterns are characterized by high resolution scanning tunneling microscopy (STM) images and successfully described by atomistic models which consider the geometric registry. Ab-initio density functional theory (DFT) simulations well reproduce the observed STM images and shed further light on the spatial corrugation of graphene and the interfacial interactions, indicating that, depending on the misorientation angle, graphene can be alternately physi- and chemisorbed or uniformly chemisorbed. The interaction is modulated periodically by the (sub)nanometer-sized moiré superstructures.

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References

[1] Vinogradov, N.A. et al., Phys. Rev. Lett., 109 (2012) 026101
[2] Murata, Y. et al., ACS Nano, 4 (2010) 6509-6514

Figures

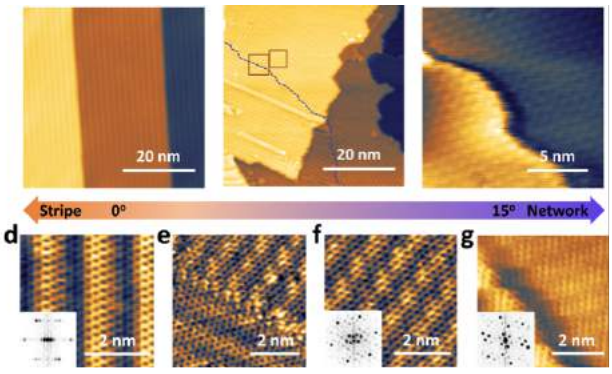

Figure 1: STM topographic images of representative graphene moirés exhibiting different periodicity and morphology (stripe & rhombic network).

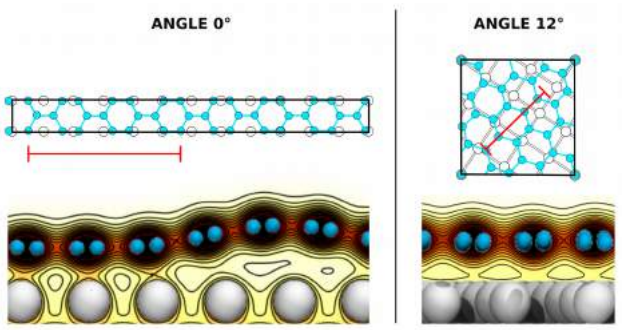

Figure 2: Total charge density plots for striped (angle 0°) and network (angle 12°) moiré structures. Charge density color scale: from white (absence of charge) to black (maximum of the charge).