Structural and electronic stability of graphene on SiC planes and facets: *Ab initio* calculations and atomic-scale imaging

Ioannis Deretzis, Filippo Giannazzo, Giuseppe Nicotra, Corrado Spinella, Antonino La Magna

CNR-IMM, VIII strada 5, 95121 Catania, Italy
ioannis.deretzis@imm.cnr.it

Abstract The interaction between graphene and its substrate can be crucial for the conservation of graphene's intrinsic electrical properties, which are necessary for the integration in devices and applications. Particular is the case of graphene thermally produced on SiC surfaces, where the structural characteristics of the graphene/substrate interface are dynamically driven during the growth process. In this work we use the density functional theory to study the properties of epitaxial graphene grown on various SiC surfaces, and compare the results with atomic-resolution structural and spectroscopic measurements. Calculations are presented for the $(6\sqrt{3}x6\sqrt{3})R30°$-reconstructed SiC(0001) surface (Si face), the (3x3)-reconstructed SiC(000-1) surface (C face) and the nonpolar SiC(11-20)/SiC(1-100) planes. We show that the formation of a strongly-bound interface buffer layer is an exclusive property of the SiC(0001) surface. The buffer layer's instability is already traceable at the (11-2n) facets of off-axis SiC(0001), where it detaches from the substrate turning into a quasi-freestanding graphene film. Moreover, our results indicate that nonpolar planes interfere less with graphene's low-energy electronic spectrum as compared to polar ones. This aspect questions the actual experimental trend and indicates new routes for the growth of graphene on silicon carbide substrates.

References

[1] I. Deretzis, A. La Magna, Phys. Rev. B, **84** (2011) 235426.
[2] F. Giannazzo *et al.*, Phys. Rev. B, **86** (2012) 235422.