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Pressure-induced phase transition of bilayer epitaxial graphene: Computations meet the experiment

Graphene exhibits unique electronic and mechanical properties. Recent AFM-based nano-indentation measurements show that two-layer graphene (2G) on SiC(0001) exhibits a transverse stiffness and hardness comparable to those of diamond [1]. Our density functional theory (DFT) calculations indicate that these mechanical properties originate from a phase transition from a graphitic to a diamond-like structure of 2G. Upon compression, a 2G film can transform into a diamond-like film in contact with SiC(0001) (Fig. 1(a)). The sp^2-to-sp^3 structural and chemical changes occur regardless of the stacking configuration (contrary to the case of a 3-layer and 4-layer graphene film) of the two graphene layers. The DFT calculations also show that a diamond-like film forms a hard contact with the SiC(0001) substrate, exhibiting an interfacial layer of bonds with a transverse elasticity as stiff as that of the substrate material. Moreover, regardless of the stacking configuration, two graphene layers buckles to form a diamond-like film, exhibiting a transverse elastic modulus ranging between 0.30 and 1.01 TPa close to that of bulk diamond. At last, I will also report classical indentation simulations, showing that a SiC(0001) substrate coated by a stiff diamond-like film yields a force vs. indentation depth curve steeper than that of the bare SiC substrate, whereas a 5-L or 2-L graphene film on SiC lead to a significant softening of the transverse mechanical response. These results are in agreement with the experimental indentation curves.

References

[1] Yang Gao*, Tengfei Cao*, Filippo Cellini, Claire Berger, Walt de Heer, Erio Tosatti, Elisa Riedo and Angelo Bongiorno, Ultra-hard carbon film from epitaxial two-layer graphene, Nature Nanotechnology, in press (2017)

Figures

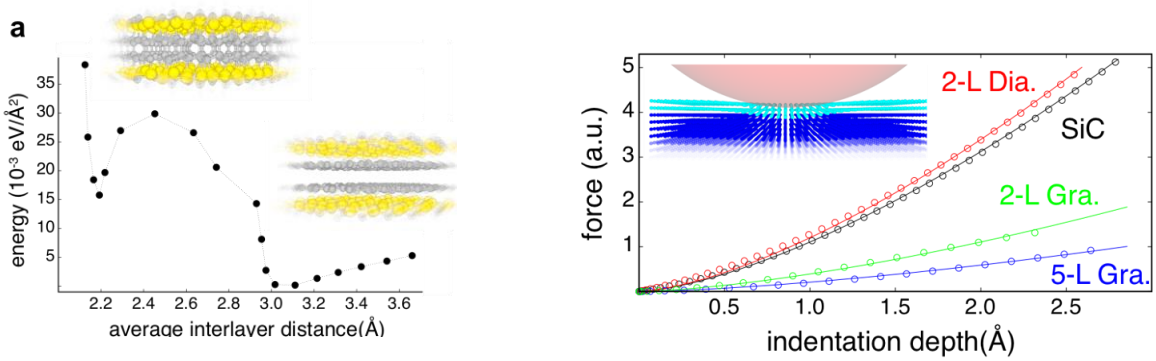

Figure 1: a) Energy per unit area obtained by DFT calculations for a two-layer graphene film sandwiched between mirroring H-SiC layers; Force vs. indentation curves obtained by using a classical scheme based on atomistic model structures and Hookean force fields.