Structure of Graphene on Ir by synchrotron X-ray scattering

G. Renaud[a] , J. Coraux [b], N. Blanc[b]

[a] *CEA, Univ. Grenoble-Alpes, INAC/SP2M, 17 rue des Martyrs, 38054 Grenoble Cedex 9, France*

[b] *CNRS, Univ. Grenoble-Alpes, Institut Néel, 25, rue des Martyrs, 38052 Grenoble 9, France*

The exceptional properties of graphene can be tailored by small structural modification, such as those induced by the epitaxy on a substrate or by defects. A combined CVD/TPG growth of graphene on Ir(111) was claimed to yield graphene of the highest quality. We have demonstrated [1] that the resulting graphene has tiny imperfections such as small biaxial strain, rotations, shears, and the coexistence of commensurate and incommensurate domains. These deviations from perfection could only be detected by X-ray diffraction. These structural variations are mostly induced by the increase of the lattice parameter mismatch when cooling down the sample from the graphene preparation temperature. Although graphene only weakly interacts with Ir, its thermal expansion was found positive [2], contrary to free-standing graphene, and was found to follow that of Ir over large temperature ranges. The detailed atomic structure of graphene was quantitatively determined by Surface X-Ray Diffraction [3]. The graphene undulation is found to be of small amplitude (0.38 Å), and to be in phase with the Ir (0.017 Å) one. The structure agrees well with recent *ab initio* calculations. The average graphene-iridium distance is 1.5 times the distance between two Ir(111) planes. The structure was also studied during growth and during the creation of defects [4]. Large strains, above 2%, are present in graphene during its growth on Ir(111) and when it is subjected to oxygen etching and ion bombardment (Fig. 1). Our results unravel the microscopic relationship between point defects and strain in epitaxial graphene and suggest new avenues for graphene nanostructuring and engineering its properties through introduction of defects and intercalation of atoms and molecules between graphene and its substrate. The organized growth of metallic nanoparticle on the graphene's moiré has also been investigated by GISAXS and X-ray diffraction.

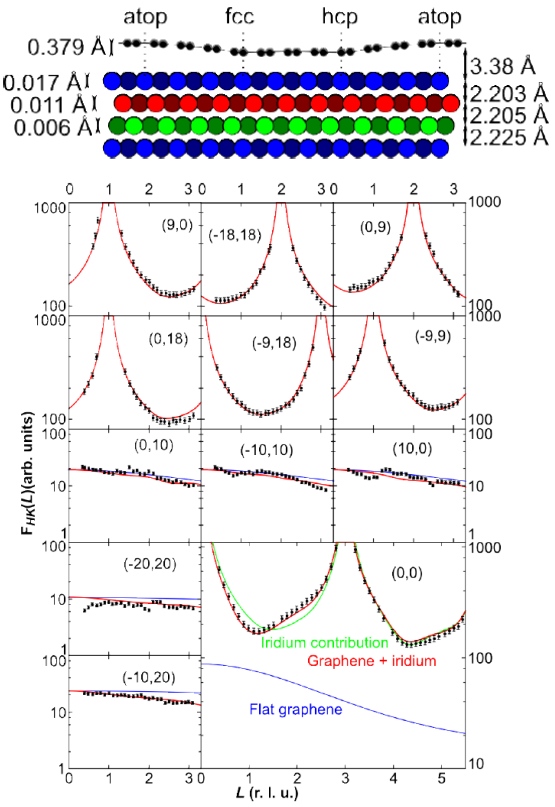

Fig. 1: Schematic side view picture of the atomic structure of graphene on Ir(111). Bottom: Rods from Ir, Gr, moiré, and reflectivity for one ML of graphene on Ir(111), together with best fits.

[+] Author for correspondence: G.Renaud@cea.fr

[1] N. Blanc et al, Phys. Rev. B 86 (2012) 235439; Phys. Rev. Lett. 111 (2013) 085501; F. Jean et al. Phys. Rev. B, **88**, 165406 (2013).