Tailoring the atomic structure and electronic properties of graphene/metal interfaces by intercalation

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The interface between graphene and the substrate plays a vital role for graphene based applications. It influences the electronic properties concerning the position and form of the Dirac cone, furthermore spin-filtering capabilities are predicted for magnetic substrates [1]. Apart from direct growth of graphene on a small number of substrates, a variety of metals can be intercalated between graphene and the substrate interface [2,3] and allow for the production of graphene on a large number of materials. In this work, we present the investigation of Ni intercalation underneath graphene on Ir(111) and Rh(111). The atomic structure and electronic properties were investigated for samples with intercalated Ni ranging from a submonolayer to few monolayers.

For Ni intercalation underneath graphene/Ir(111), scanning tunneling microscopy shows large monolayer thick areas of intercalated material accumulated at step edges. These areas show a strongly increased moiré corrugation as well as a decreased average distance of graphene from Ni/Ir(111) compared to Ir(111). The stronger corrugation in conjunction with considerable changes in the electronic structure measured by the photoemission spectroscopy suggests an increased bonding between graphene and Ni. The details of the atomic structure and electronic properties are discussed in the frame of recent DFT calculations of graphene/Ni/Ir(111).

For Ni intercalation underneath graphene/Rh(111) [2], we observe the formation of epitaxial nanoislands underneath graphene, which are scattered across the substrate terraces. The size and shape of nanoislands is strongly influenced by the local spatial variation of the graphene-Rh bonding strength involving size selection according to the moiré periodicity. Here, no considerable changes in bonding strength are observed as compared to graphene/Ni/Ir(111).

In both systems, we identify the intercalation paths to be via diffusion through either pre-existing defects in graphene, or metal-generated defects followed by the defect healing of the graphene lattice. For intercalation of Ni underneath graphene/Ir(111) large patches of material, often in the vicinity of step edges, are found and suggest long diffusion lengths of material at the interface of graphene and Ir(111) This is not the case for graphene/Ni/Rh(111), where the strongly bound bridge sites act as diffusion barriers. Similar diffusion barriers can be achieved after intercalation of more than one monolayer of Ni.

References

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Figures

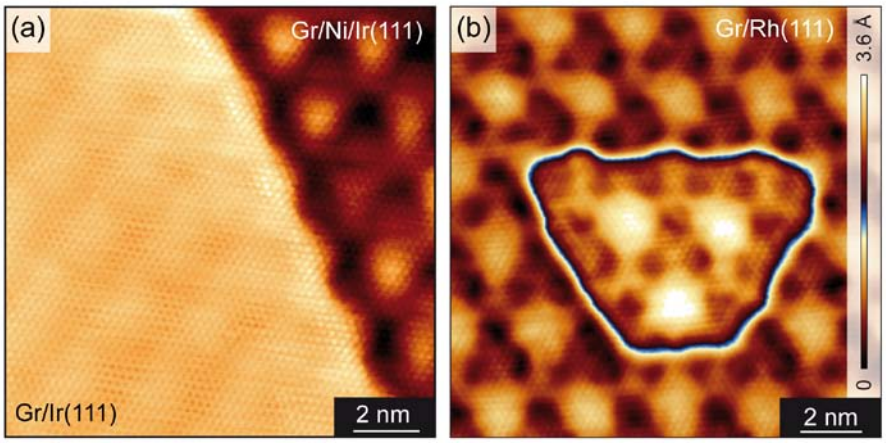

Fig. 1: (a) STM topograph of intercalated Ni underneath graphene/Ir(111). Intercalated material shows increased moiré corrugation and accumulates at step edges. (b) STM topograph of intercalated Ni underneath graphene/Rh(111). Strongly bound areas of the graphene/Rh(111) moiré cell act as diffusion barriers for material, eventually forming intercalated islands with size-selection.