

Effects of the nanoscale structural modulation on graphene's electronic structure

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Structurally modulated graphene presents a new variety of this 2D material which offers a possibility of electronic band engineering and promises to extend a wide range of possible applications of graphene from straintronics, optoelectronics and spintronics, coatings, sensors for batteries, etc. [1–9] Motivated by these prospects, and a small number of experimental realizations of the modulated graphene systems, we have synthesized and studied epitaxial graphene on stepped Ir(332) substrate.

The system was studied with a comprehensive set of experimental techniques which gave the insight into structural characteristics (scanning tunneling microscopy (STM) and low energy electron diffraction (LEED)) and electronic band structure (angle-resolved photoemission spectroscopy (ARPES) and density functional theory (DFT)).

The graphene on Ir(332) caused a severe, yet reversible, surface restructuring, consisting of formation of large (111) terraces and (331) step bunches, giving the substrate and graphene a new periodicity. We found that the new periodicity as well as the graphene rotation can be controlled through variation of growth parameters. Measurements of the electronic band structure of the graphene on (111) facets showed the Dirac cone anisotropy with a severe Fermi velocity reduction in the direction parallel to the step edges (Fig. 1) consistent with the theory [10–12]. We have attributed this anisotropy to the 1D periodicity present in the system. Additionally, the graphene π band is also tilted, which is likely an affect of graphene buckling due to its periodical is bending across step edges. ARPES measurements of π band corresponding to the graphene on (331) facets revealed a strong n-type doping as well as band gap opening in the vicinity of the Ir surface states indicating possible hybridization. The DFT calculations showed that the graphene binding is strongest on the step edges, where graphene is essentially anchored. At step edges a severe orbital mixing occurs, and this local graphene chemisorption drives the surface restructuring in competition with the strain present in the system. The explanation of the graphene mediated surface restructuring process is general enough to incorporate all systems with van der Waals interaction.

Our findings demonstrate a viable route to alter epitaxial graphene's electronic structure by means of strain and van der Waals interaction, and give an explanation of the surface restructuring process. [13]

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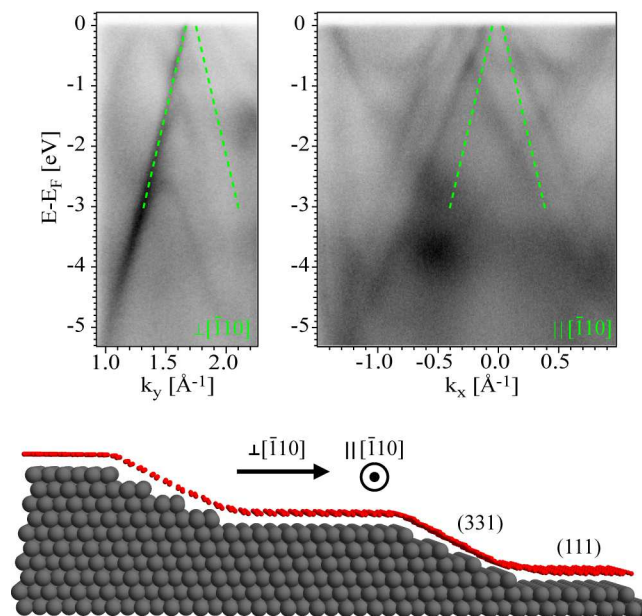


Figure 1: ARPES spectra of graphene on restructured Ir(332) recorded in direction perpendicular and parallel to the step edge direction. Green lines represent linear fit of the Dirac cone in the perpendicular direction. Surface model shows relevant directions and facets.