Rotated Domains in Chemical Vapor Deposition-grown Monolayer Graphene on Cu(111): An Angle-resolved Photoemission Study

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Copper is considered to be the most promising substrate for the growth of high-quality and large area graphene by chemical vapor deposition (CVD), in particular, on the (111) facet. Because the interactions between graphene and Cu substrates influence the orientation, quality, and properties of the synthesized graphene, we studied the interactions using angle-resolved photoemission spectroscopy. The evolution of both the Shockley surface state of the Cu(111) and the p band of the graphene was measured from the initial stage of CVD growth to the formation of a monolayer. Graphene growth was initiated along the Cu(111) lattice, where the Dirac band crossed the Fermi energy (E_F) at the K point without hybridization with the d-band of Cu. Then two rotated domains were additionally grown as the area covered with graphene became wider. The Dirac energy was about 0.4 eV and the energy of the Shockley surface state of Cu(111) shifted toward the E_F) by 0.15 eV upon graphene formation. These results indicate weak interactions between graphene and Cu, and that the electron transfer is limited to that between the Shockley surface state of Cu(111) and the p band of graphene. This weak interaction and slight lattice mismatch between graphene and Cu resulted in the growth of rotated graphene domains (9.6° and 8.4°), which showed no significant differences in the Dirac band with respect to different orientations. These rotated graphene domains resulted in grain boundaries which would hinder a large-sized single monolayer growth on Cu substrates.

Keywords: Graphene, Cu, Band structure, monolayer, Domain

The Interfacial Electronic Structure of Organic–organic Heterojunction: Effect of Molecular Orientation

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The orientation of the constituent molecules in organic thin film devices can affect significantly their performance due to the highly anisotropic nature of π-conjugated molecules. We report here an angle dependent x-ray absorption study of the control of such molecular orientation using well-ordered interlayers for the case of a bilayer heterojunction of chloroaluminum phthalocyanine (ClAlPc) and C60. Furthermore, the orientation-dependent energy level alignment of the same bilayer heterojunction has been measured in detail using synchrotron radiation-excited photoelectron spectroscopy. Regardless of the orientation of the organic interlayer, we find that the subsequent ClAlPc tilt angle improves the π-π interaction at the interface, thus leading to an improved short-circuit current in photovoltaic devices based on ClAlPc/C60. The use of the interlayers does not change the effective band gap at the ClAlPc/C60 heterointerface, resulting in no change in open-circuit voltage.

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Keywords: x-ray absorption spectroscopy, photoemission, synchrotron-radiation, organic semiconductors