The Diamond (111) Surface Reconstruction and Epitaxial Graphene Interface

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A rejuvenated interest in diamond as a state-of-the-art electronic material has occurred over the last couple of decades as its potential for use in emerging quantum information and sensing technologies becomes apparent. The growing demand for miniaturisation has also led to increased interest in the nanoscale properties of diamond and the production of diamond-graphene (sp3 – sp2) interfaces. However, fundamental studies of the diamond (111) surface electronic structure remain incomplete and controversy surrounding the metallic[1] or semiconducting[2] nature of the (2×1) surface reconstruction remains unresolved. We therefore follow the evolution of the diamond (111) surface electronic and physical structure as it undergoes reconstruction and subsequent graphene formation with angle-resolved photoemission spectroscopy, low energy electron diffraction, and compare to complementary density functional theory calculations.

The studies begin on the hydrogen terminated H:C(111)-(1×1) surface, proceeding to the C(111)-(2×1) surface reconstruction that occurs following detachment of the surface adatoms at 920 °C. We then continue through to the liberation of the reconstructed surface atoms into a free-standing monolayer of epitaxial graphene at temperatures above 1000 °C. Our results show that the C(111)-(2×1) surface is metallic as it has electronic states that intersect the Fermi-level. This is in strong agreement with a symmetrically π-bonded chain model and should contribute to resolving the controversies that exist in the literature surrounding the electronic nature of this surface. The graphene formed at higher temperatures exists above a newly formed C(111)-(2×1) surface and appears to have little substrate interaction as the Dirac-point is observed at the Fermi-level. Finally, we demonstrate that it is possible to hydrogen terminate the underlying diamond surface by means of plasma processing without removing the graphene layer, allowing for tuneable substrate interactions at the graphene-semiconductor interface[3].

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