Atomic and topographic corrugations of graphene on 6H-SiC(0001) derived from Grazing Incidence Fast Atom Diffraction

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Abstract

The exceptional properties of graphene and the prospect to use it as the new material for next generation micro- and nano-electronic devices are still waiting for major advances in the production methods in terms of scaling and cost. Current efforts to develop an effective process for producing large samples of high quality graphene could be made easier if characterization techniques, which provide reliable information on sensitive properties such as geometric corrugation, domain size, number of layers and their relative orientation, were able to operate in situ or if possible in real time during the growth process. Supported graphene most often exhibits a Moiré superstructure that originates from local anchoring of the graphene layer onto the substrate. The corresponding corrugation, of geometric origin and which provides a good estimate of the coupling strength between the carbon layer and the substrate, has a strong influence on the graphene properties. For instance the relationship between corrugation and thermal stability of graphene/Re(0001) has been demonstrated [1]. Yet precisely quantifying the corrugation of the Moiré has not become systematically accessible. As an illustration, figures of the superstructure corrugation of graphene grown on Ru(0001) differ substantially whether you consider density-functional-theory calculations [2], STM [3], XRD [4] or Helium Atom Scattering (HAS) [5].

Here we propose another method, Grazing Incidence Fast Atom Diffraction (GIFAD) [6,7], to reliably derive both atomic and geometric corrugations with high sensitivity. Physically, GIFAD is very similar to the technique used by Borca et al. [5]. However GIFAD uses helium atoms in the keV energy range in a scattering geometry comparable to that of RHEED; the diffraction pattern is recorded at once on a position sensitive detector and the image captured by a CCD camera.

Figure 1 shows diffraction patterns measured with 300 eV He on a single layer graphene grown on 6H-SiC(0001). The intrinsic atomic corrugation is observed along the zig-zag (right-hand side) direction, while the topographic corrugation of the Moiré superstructure is observed along the armchair (left-hand side) direction. We measure a period of 2.13 Å for graphene atomic structure; the period measured along the armchair direction yields a value of 16 Å, i.e. the 13x13 phase of graphene, which is commensurate with the $\bar{}$ $\bar{}$ of the SiC(0001) [8].

GIFAD probes the interaction potential, averaged along the beam direction, between the incident He atom and the surface. We describe the He-surface interaction using a Lennard-Jones He-C pair-wise potential [9] that has been optimized to reproduce HAS data on graphite. We have considered a graphene layer frozen at its equilibrium position [10] and calculated the diffracted intensities with a close coupling code described in [11]. Without any adjustment, the calculated diffraction probabilities in the zig-zag direction are comparable to the measured values, thus providing confidence on the validity of the potential.

The Moiré structure is introduced by modulating the atom vertical positions on a 13x13 superlattice according to a model-corrugation adjusted to the *ab initio* data reported by Varchon et al. [12]. In this case, the calculated diffraction probabilities along the armchair direction do not reproduce the experimental data. However a good agreement is achieved if the Moiré corrugation from Varchon et al. is scaled by a factor 0.7. Figure 2 shows the atomic structure that best fits our diffraction data, the corresponding geometric corrugation is 0.275 $\pm$0.02 Å.

These results demonstrate the capability for GIFAD for resolving the structure of epitaxial graphene. The GIFAD sensitivity, together with its ability to operate at high temperatures makes this technique a good candidate for real time monitoring of graphene growth.

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Figures

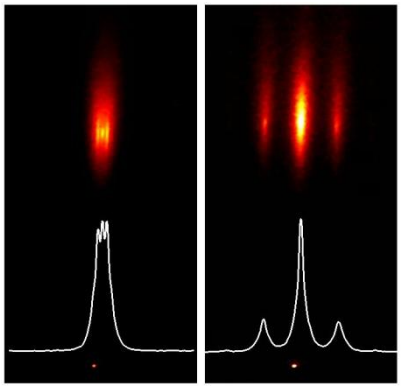

Fig. 1. Diffraction patterns measured with 300 eV He along the armchair (left) and ziz-zag (right) directions. The bottom profile is the horizontal projection of the diffraction pattern.

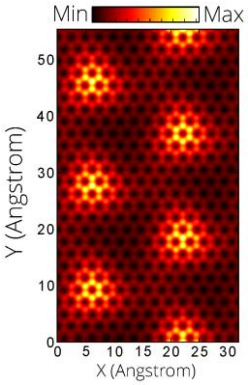

Fig. 2. Constant-height image of the He-graphene potential-map following optimization on the experimental diffraction data.