Experiment Report Form

ESRF	**Experiment title:** Structural and electronic properties of graphene on a model support: C/Ir(111)	**Experiment number**: SI-1885
Beamline: ID32	**Date of experiment**: from: 24.4.2009 to: 4.5.2009	**Date of report**:
Shifts: 17	**Local contact(s)**: Jörg Zegenhagen	*Received at ESRF:*

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Report:

Epitaxial growth on transition metal surfaces is a promising method for graphene preparation. Especially on Ir(111) we have previoulsy proven a high degree of graphene's structural quality [Coraux2008, NDiaye2008], while its electronic structure is largely identical to the one of free graphene [Pletikosic2009]. These results lead to the assumption, that graphene on Ir(111) is only weakly bound to the substrate through Van-der-Waals-forces. In addition, DFT predicts interesting effects in this system, e.g. a buckling of the graphene layer or a rehybridization induced by growth of additional Ir leading to the formation of well-ordered extended cluster lattices [NDiaye2006,Feibelman2008]. These assumptions can be substantiated by a determination of the distributions of vertical bond distances between the Ir substrate and the graphene overlayer as the bond distance is a measure of the bond strength and its distribution contains information about buckling and rehybridization effects. Furthermore, such a measurement would help to assess the validity of new DFT functionals taking vdW-forces explicitely into account.

To determine the bond distances we performed *in situ* XSW measuremtents of graphene on Ir(111). In addition we investigated the changes in the bond pattern introduced by the growth of highly ordered superlattices of Ir-clusters on top of the graphene. Experimentally, the XSW-UHV-chamber at the beamline ID32 was supplemented with additional equipment necessary for the proposed experiments, including a special sample holder, a calibrated, very clean Ir-evaporator, and a quartz crystal balance. The use of a special sample holder using e-beam heating was required by the high temperatures needed to prepare well ordered graphene on Ir(111) while maintaining a low background pressure. A first test of the sample holder in the XSW-chamber under UHV-conditions failed due to loss of contact to the filament, necessitating a second bake out. After modification of the holder, the high temperatures needed could be reached (> 1200 °C), showing that the new sample holder can be used for this kind of experiments also for future beamtimes. After this, the gas inlet system of the chamber wich we used to supply ethene for graphene growth showed a leak in one of the dose valves, leading to an accidentially venting of the chamber, requiring a third bakeout. As a consequence of these experimental problems, the first ten allocated shifts could not be used for measurements. The last shift was cancelled due to MDT. In the following the experimental results of the remaining 7 shifts are reported.

We have prepared graphene on Ir(111) in two different coverages (0.4 ML, 0.6 ML) using temperature programmed growth (TPG), see e.g. [Coraux2009]. For these systems we have performed an XSW-analysis using the (111) diffraction spot.

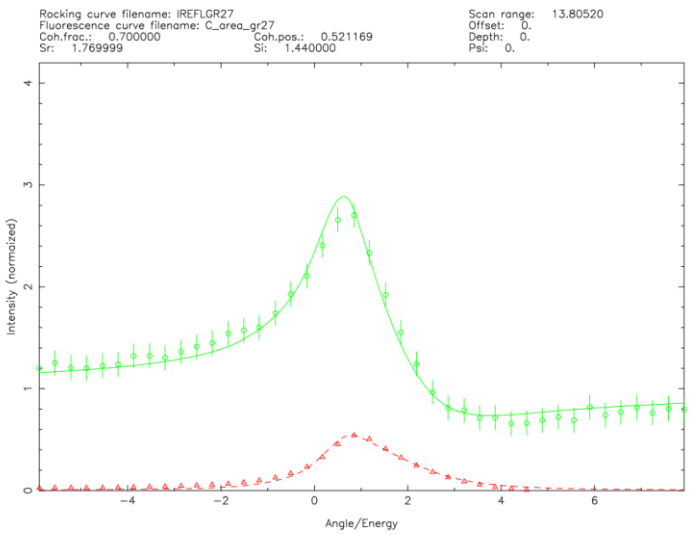

Fig 1.: XSW-scan (C1s) of 0.6 ML graphene on Ir(111)(green) together with the reflectivity curve (red). Lines are fits to the data.

A coverage of 0.4 ML graphene shows a LEED-pattern equivalent to the one observed in our home lab after a comparable preparation. The XPS measurements revealed a C1s-peak with E_B=284.2 eV, identical to the value published recently [Preobrajenski2008]. Via XSW the bonding distance and the height variation due to a buckling of the graphene layer could be determine accurately (see Fig. 1 for an example of an XSW scan). The bond distance is significantly smaller than the one predicted using DFT [Feibelman2008] which is understandable since in this calculation vdW-forces have been neglected. The degree of buckling is slightly larger than in the DFT-calculations.

Upon deposition of Ir metal on top of the graphene layer, the LEED-pattern changes as observed previously. A splitting of the C1s-peak caused by a chemical shift due to the adsorption of Ir is not observable with the resolution achieved. However, a significant broadening of the peak and a slight shifitng of the peak position was found. The XSW-analysis reveals that the average bonding distance is almost unaltered when compared to the bare graphene layer, but the height distribution is much broader. This finding is in agreement with the predictions based on DFT.

In conclusion the beamtime was successful and yielded important parameters for graphene on Ir(111) with and without clusters. The evaluation of the data is still in progress and a further refinements of the results obtained is expected. A scientific publication based on these findings is in preparation. Furthermore, the experimental problems solved at the beginning of the beamtime will make future beamtimes for this system (which we will apply for) much easier, so that based on the findings presented here, further, more detailed studies are well possible.

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