ESRF	**Experiment title:** Investigation of the interaction strength at the organic-organic interface	**Experiment number**: SI-2277
Beamline: ID 32	**Date of experiment**: from: 18/04/2011 to: 27/04/2011	**Date of report**: 29/08/2012
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Report:

1. Introduction

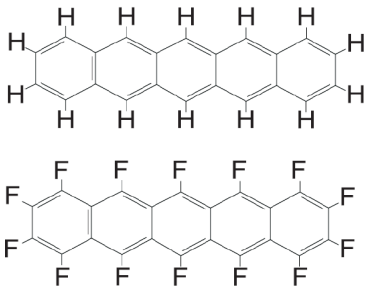


Figure 1: Chemical structure of pentacene (top) and perfluoro-pentacene (bottom).

For the this beamtime we proposed to investigate the interaction strength between organic molecules using the XSW technique. For this purpose, we chose perfluoropentacene (PFP) on pentacene (PEN) on Cu(111)‡, see Fig. 1. It was shown by Koch et al. [1] that both molecules adsorb on Cu(111) in a lying geometry, but the PEN molecule has a significant lower bonding distance than its fluorinated counterpart. Additionally, the bending of the fluorine atoms above the carbon core results in a distortion of the molecule and hence in a permanent dipole moment influencing the workfunction of this sample.
On SiO_2, films prepared by co-evaporation of PEN and PFP showed a regular lattice of alternating molecules caused by quadrupole interaction between PEN and PFP [2].

‡ Because of competing efforts by other collaborations we decided not to use the bilayer system zinc-phthalocyanine on PTCDA on Cu(111), which we suggested in the proposal.

2. XSW measurements of PEN on Cu(111)

First, we prepared a monolayer of PEN on Cu(111). During evaporation of PEN we held the temperature of the substrate at around 450 K where the second layer of PEN starts to desorb [3]. Then we performed XSW accompanied by XPS measurements. Our XSW results are in good agreement with earlier results [1]. A representative XSW scan of carbon is displayed in Fig. 3.

3. XSW measurements of PFP on PEN on Cu(111)

Second, we evaporated a submonolayer of PFP on PEN/Cu(111) followed by XSW and XPS measurements. The XPS signal of carbon can be fitted with 3 peaks (Fig. 2). The biggest peak corresponds to the carbon of PEN, whereas the two smaller peaks belong to PFP, the one with higher binding energy emerging from the C-F, the other from the C-C binding within the molecule. Such a detailed XPS analysis allows to distinguish the photoelectron yield of carbon of the PEN from the carbon of PFP and therefore a separate determination of the bonding distance of the carbon core of PEN and PFP of the bilayer system.

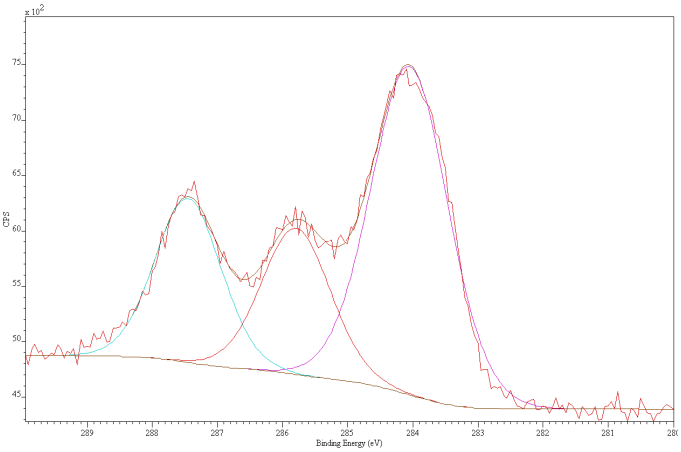


Figure 2: C1s spectrum of the bilayer system PFP on PEN on Cu(111).

In order to avoid beam damage of PFP we had to reduce the time of exposure to the X-ray beam. We solved this challenge by splitting one XSW scan into four segments which were measured at different spots. Additional scans of the reflectivity were taken at each spot for reference. For the analysis we stitched the individual scans together. A typical XSW measurement of the bilayer PFP on PEN on Cu(111) can be seen in Fig. 3. We can conclude by looking at the coherent fraction of the C1s signal that there is no systematic in-plane intermixing of PEN and PFP. Otherwise there would be no decrease in the coherent fraction of the integrated (PEN plus PFP) carbon signal compared to the individual components. Analyzing the coherent position we see that the bonding distance of the carbon of

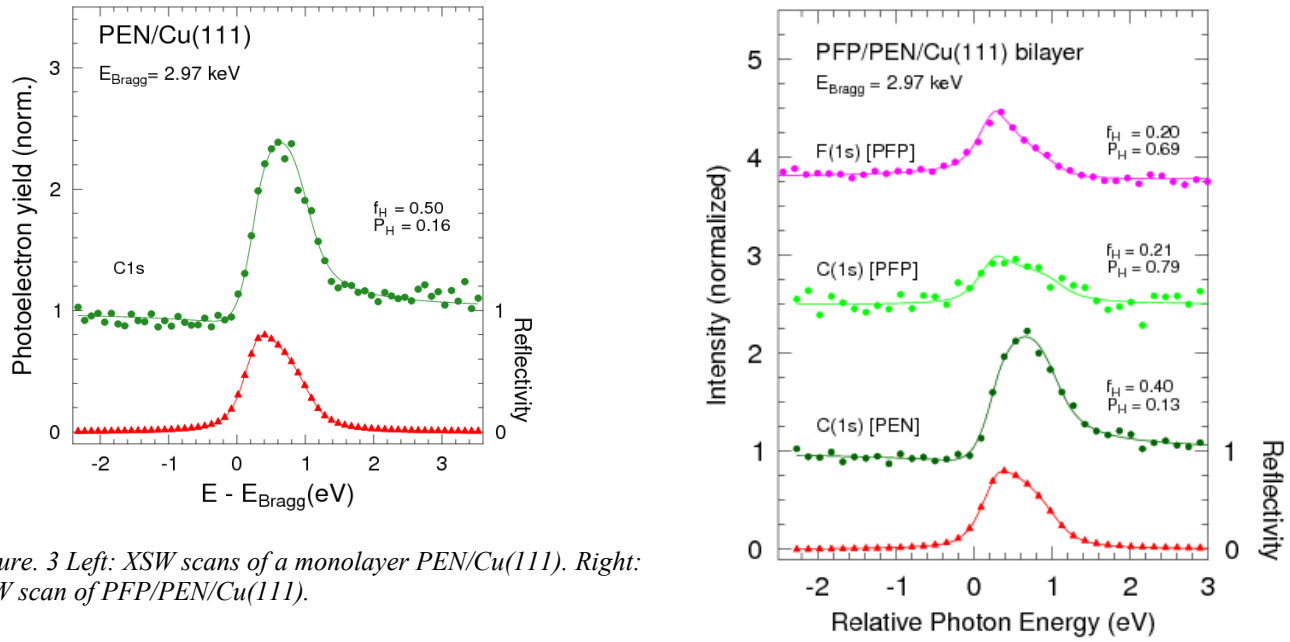
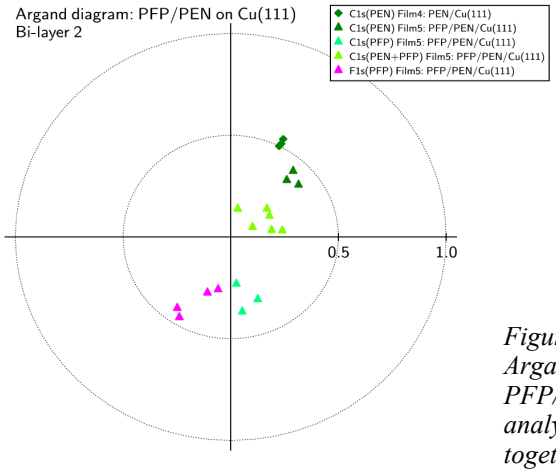


Figure. 3 Left: XSW scans of a monolayer PEN/Cu(111). Right: XSW scan of PFP/PEN/Cu(111).

PEN in the bilayer is slightly reduced relative to case where only PEN adsorbs on Cu(111). The carbon atoms of the PFP molecule are 3.37 A above the PEN layer, which is a typical inter-planar distance of the bulk material [4]. In contrast to the system PFP on Cu(111), there is now the situation that fluorine atoms are bent downwards towards the substrate. These results are visualized schematically in Fig. 4.



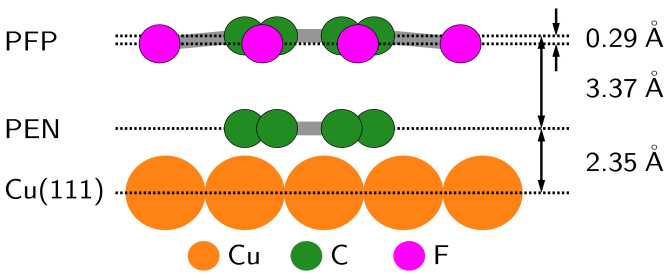


Figure 4: Right: Sketch of the bilayer PFP on PEN on Cu(111). Left: Argand diagram: XSW measurements of PEN/Cu(111) (diamond) and PFP/PEN/Cu(111) (triangle). The carbon of the bilayer system was analysed separately for PEN (dark green), PFP (turquoise) as well as both together (light green) and fluorine (pink).

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