ESRF	**Experiment title:** Surface X-ray diffraction study of molecular structure, orientation and substrate interaction at the pentacene/Au(111) systems	**Experiment number**: **SI-1572**
Beamline: ID3	**Date of experiment**: from: 12 ott 2007 to:20 ott 2007	**Date of report**: 26 febr 2007 *Received at ESRF:*
Shifts: 21	**Local contact(s)**: Didier Wermeille	

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Report:

The SXRD experiments were performed at the ID03 beamline. Our aim was to perform Surface X-ray diffraction measurements to enlighten the Pn effect after deposition on the Au(111) system. The system was characterized previously in our laboratory by electron spectroscopies (UPS, NEXAFS) and LEED. The coverage of Pn at ID3 was calibrated by means of Auger spectroscopy.

The clean Au herringbone structures remain measurable (Fig. 2) indicating a weaker perturbation of the Au substrate with respect to the previous fullerene case.
We measured the CTR in order to get the information on the number of substrate atoms involved in the reconstruction (incommensurate, so very difficult to be measured).

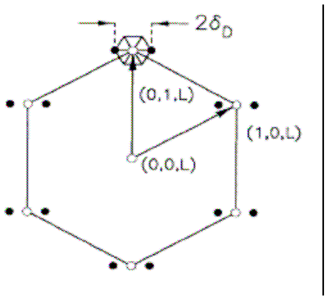

Figure 1 Clean Au(111)
[ref Phys. Rev. B 43, 4667 (1991)]

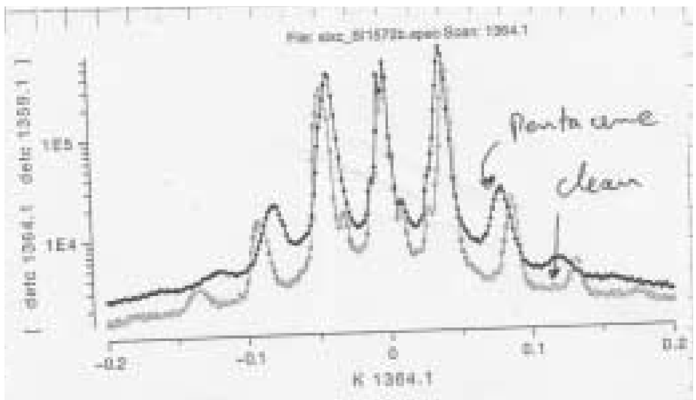

Figure 2
Circle scan shows Au(111) satellites peaks due to the clean herringbone structure. These wiggles result shifted after Pn deposition

Pentacene deposition was performed following the same procedure used in our lab. STM measurements of molecular ordering of pentacene on Au(111) films show that the phase diagram is extremely rich, exhibiting a large number of coverage dependant ordered structures.[1]. Moreover for multilayer films, discrepancies are found in the interpretation of data on growth of the second and subsequent layers [2], where STM measurement suggest a unique widely spaced periodic row structure, with a 61 ± 5 Å spacing.

Following the procedure of the previous a 4x4 multilayer structure was obtained. At room temperature the 4x4 multilayer structure did not remain for a time longer than few minutes. We cooled down the sample and mounted shutters in order to limit the exposition of the sample to the x-ray beam to only the acquisition time. The 4x4 survived longer. We succeeded in measuring the CTR of the substrate for the 4x4 Pn/Au(111). After 8 hours of Pn 4x4 layer exposed to the X-ray beam the wiggles resulted smeared out but their position in K scan remain that of the 4x4 layer. We refreshed the 4x4 Pn layer frequently verifying the disruption versus time behavior.
Moreover we verified the very rich phase diagram of Pn/Au(111) and different superstructures could be obtained. In particular for a Pn deposition at 40 °C we found a incommensurate superstructure of the first ML of Pn. All the reconstruction measured so far presented weak detectable peaks and were related to incommensurate periodicity along the h direction. The gold CTR did not appear perturbed after the molecular deposition, indicating that the structure along the z axis was not perturbed, in agreement with the weak interaction of the Pn molecule with Au substrate.
This behaviour is related to the weak bond between the Pn and the Au(111) substrate, weaker than the tetracene or pentacene on Ag(111) [our ref].
The substrate wiggles related to the herringbone structure of the Au(111) have been measured (Fig.2). The good quality of the Au(111) clean surface is related to the fact that wiggles up to the fourth order could be measured (dark line in the figure). After deposition of a single monolayer, the periodicity of the herringbone Au(111) wiggles changed (Fig.2). It results that the periodicity after Pn deposition changed from 23 to 25 rows of substrate involved in the herringbone structure.
The main result was that the substrate gold layer underneath a single Pn layer does not show any sign of the Pn reconstruction indicating a weaker perturbation of the Au substrate with respect to the fullerene case deposition [esrf highlights 2007]. We infer that the change in the wiggles periodicity can be related to "electrostatic" reason at the interface. Theoretical analysis should model this result.
The data analysis and the writing of the relative paper are in progress.

References

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[2] G. Beermink, T. Strunskus, G. Witte, C. Woell Appl. Phys. Lett. 85, 398 (2004); J. H. Kang, X. Y. Zhu, Appl. Phys. Lett. 82, 3248, (2003).