ESRF	**Experiment title:** Binding site, orientation, and structural coherence of PTCDA molecules on Ag(111)	**Experiment number**: SC-698
Beamline: ID 32	**Date of experiment**: From: April 04, 2000 to: April 14, 2000	**Date of report**: April 19, 2000
Shifts: 18	**Local contact(s)**: J. Zegenhagen / B. C. C. Cowie	*Received at ESRF:*

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Report:

As outlined in the proposal, this experiment has focussed on an x-ray standing wave (XSW) and x-ray photoelectron spectroscopy (XPS) study of a model system for organic molecular beam epitaxy (OMBE), namely PTCDA (3,4,9,10-perylenetetracarboxylic dianhydride, C24H8O6) on Ag(111). The bonding distance, d, of the flat PTCDA molecule on the Ag(111) surface is of prime importance for the understanding of this van-der-Waals-driven epitaxy, and it could be successfully determined by XSW. ***Since this report is submitted only one week after the experiment, the analysis is not yet finished. However, after a first screening of the data, we can consider the experiment to be very successful. Below we give a preliminary summary of the results:***

1) From the shape of the XSW signal (Fig.1) detected by C(1s) XPS, we estimate the bonding distance, d, to correspond to a coherent position, P(111), of about 1.2, i.e. 2.8 Angstroms.

2) The coherent fraction appears to be relatively high, which is presumably due to the nature of the flat and rigid molecule, which is very suitable for XSW studies, and the appropriate preparation conditions.

3) Besides exploiting the Ag(111) reflection, we also studied the XSW signal from the Ag(222) reflection. Despite the difficult experimental conditions (including the need to apply a bias voltage of 2kV to the sample for the detection of C(1s) photoelectrons and the low XPS cross-section for higher-energy x-rays), we were able to record a complete data set. Due to technical instabilities related to the bias voltage, this could unfortunately not be continued. Nevertheless, the existing (222) XSW data set will significantly improve the precision of our structure determination.

4) The separate detection of C and O enabled us to investigate the coherent position and fraction of these species independently.

5) The observed peak splitting in the O(1s) XPS signals (Fig.2) with high resolution in the monolayer regime offers the possibility to determine the adsorption site for different chemical shifts. For a molecular semiconductor like PTCDA, for which in many applications the electron transfer from a metal electrode is crucial, this could strongly promote the fundamental understanding and the optimization of related devices. Depending on coverage, also the C(1s) levels were found to exhibit a splitting.

6) The XSW and XPS studies were performed at different temperatures (-110 deg C, 25 deg C, and 170 deg C) to determine differences in d. Different temperature cycles were followed, both for the preparation temperature and the XSW measurement temperature in order to identify small, but important differences in the adsorption state, for which we have evidence in combination with supporting data from other techniques (vibrational spectroscopy).

7) Finally, we believe our data can contribute to a better understanding of the XSW technique itself, in that we have recorded XSW data both with XPS and with Auger electron detection, for highly coherent monolayers as well as for intentionally incoherent multilayers, as recently discussed by Woodruff and coworkers (PRL 84 (2000), 2346). The comparison of these data sets will help to address the question of the strength of non-dipolar contributions in the XPS-detection of XSW.

We also wish to acknowledge the excellent collaboration with the ESRF scientists B.C.C. Cowie and J. Zegenhagen, which made this challenging experiment a success.

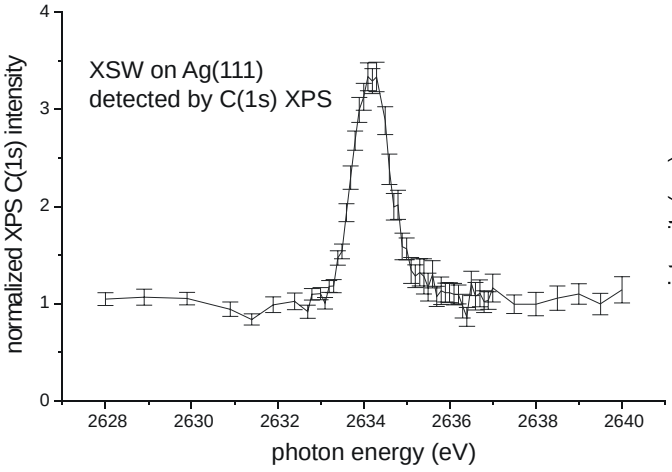

Fig.1: XSW scan detected by XPS from C(1s).

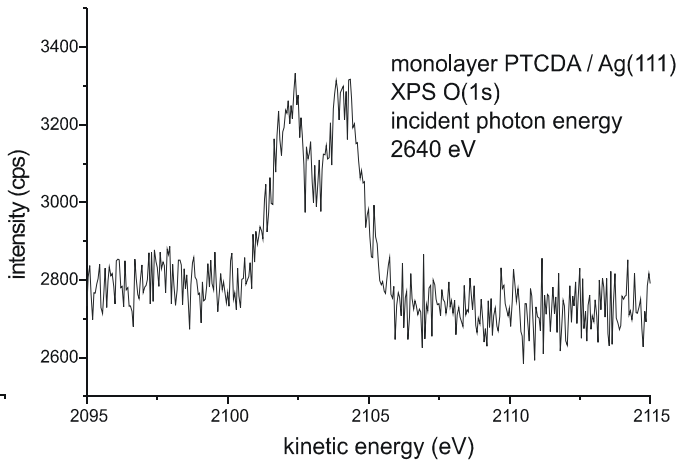

Fig.2: XPS of O(1s).