ESRF	**Experiment title:** **Adsorption of organic molecules on metal surfaces**	**Experiment number**: **SI 748**
Beamline: ID-32	**Date of experiment**: from: 28.01.2002 to: 05.02.2002	**Date of report**: 21.09.2002
Shifts: 24	**Local contact(s)**: **Bruce Cowie / Jörg Zegenhagen / Tien-Lin Lee**	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

C. Kumpf*, J. Stanzel*, W. Weigand*, E. Umbach
Deptartment for Experimetal Physics II, University of Würzburg,
Am Hubland, D-97074 Würzburg, Germany

H.L Meyerheim*,
Max-Planck Institut für Mikrostrukturphysik,
Weinberg 2, D-06120 Halle, Germany

Report:

In the last years basic research in the field of organic semiconductors was often focussed on obtaining high electroluminescent yield, high charge carrier mobility and superconductivity, because these effects enabled the development of, e.g., light-emitting devices, field effect transistors and solar cells based on organic materials [1]. But even though surface and interface effects are dominant in such devices, detailed knowledge about their geometric structure and about the influence on their electronic properties are rarely available.

In the beamtime reported here we have started to investigate a model-system for aromatic adsorbates, namely a commensurate monolayer (ML) of NTCDA on Ag(111) using the normal incidence x-ray standing wave (NIXSW) technique. This system shows a very unusual phase transition, an order-disorder phase transition upon ***cooling*** below 140 K which was firstly found in SPA-LEED and NEXAFS experiments. These measurements suggested more weakly bonded molecules for the disordered low temperature (LT) phase compared to a chemisorbed state in the ordered room temperature (RT) phase. Since this effect should be accompanied by a significant change of the bonding distance between the Ag surface and the adsorbed NTCDA molecule we planned to perform NIXSW measurements on both, the RT and the LT phase. But due to technical problems with the sample cooling we did only reach a temperature of about 160 K which is insufficient to examine the LT phase. Thus the experiment could be performed at RT only. However, the RT results are very promising. From O1s and C1s photoelectron yield measurements we were able to evaluate the exact distance of the molecule to the surface, a result which is not self-evident since the molecule consists of light elements only. Exemplary NIXSW measurements and corresponding fit calculations using a code written by Woodruff *et al.* and modified by Kilian [2] are shown in Fig. 1. The O1s electron

yield for the relaxed ML phase and the C1s yield for the compressed phase are plotted in the left and right part of the figure, respectively, the corresponding fit parameters are shown in Table 1. In each of the phases the O1s and C1s give – within experimental errors – the same result for the coherent position, i.e., for the distance between the surface and the carbon and oxygen atoms, respectively. On the other hand there is a significant difference between relaxed and compressed phase, the coherent position is higher for the relaxed phase. On one hand these results are very interesting by themselves because they can be compared to those by the very similar but larger molecule PTCDA on Ag(111) obtained by Schreiber *et al.* which yielded a significantly smaller distance [3]. On the other hand they demonstrate, that the accuracy of the measurements is indeed high enough to indicate a change of the bonding distance caused by the LT phase transition, if present. It is therefore an urgent goal to perform the LT NIXSW experiments, after the cooling system of the sample manipulator has been improved. The expected results would give essential insight into the mechanism and the driving force of this unusual order-disorder phase transition.

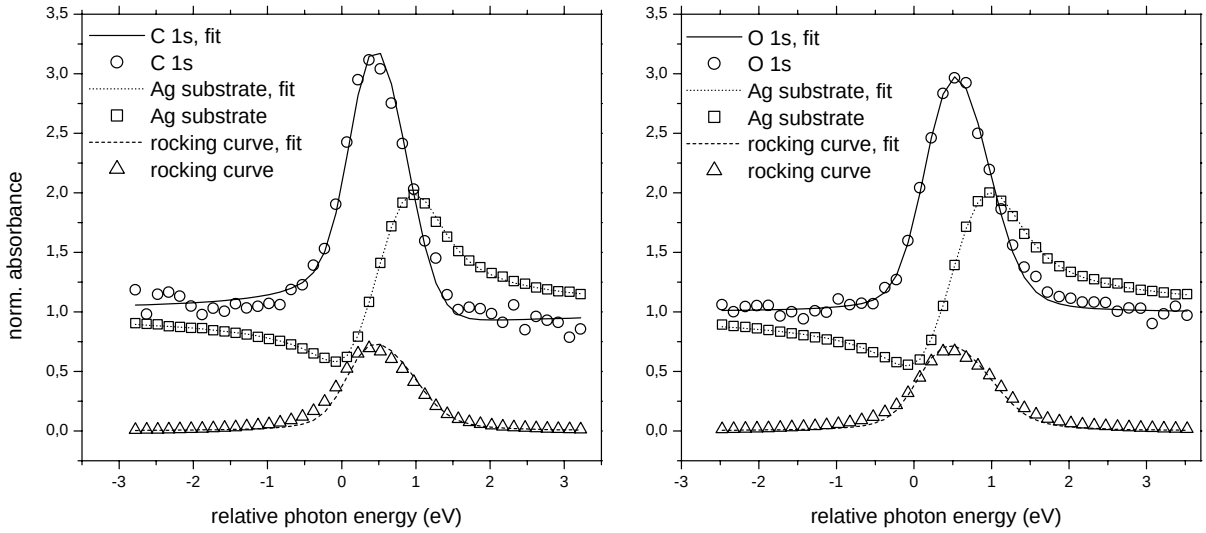

Figure 1: NIXSW measurements and corresponding fit curves for a relaxed (left) and compressed (right) monolayer structure of NTCDA on Ag(111) at room temperature. The relative absorption versus photon energy curves (relative to the Bragg energy of 2.625 keV) are shown together with the rocking curves of the Ag(111) Bragg reflection and the substrate curve derived from the photoelectron background.

Table 1: Fit results for the photoelectron yield NIXSW measurements shown in Fig. 1.

	adsorbate		substrate	
	coh. position	coh. fraction	coh. position	coh. fraction
relaxed ML (O1s)	3.02 Å	0.89	2.36 Å	0.87
compressed ML(C1s)	3.14 Å	1.00	2.36 Å	0.81

[1] J.H. Schön *et al.*, Nature **408**, 549 (2000), **406**, 702 (2000), M. Wohlgenannt *et al.*, Nature **409**, 494 (2001); M. Gross *et al.*, Nature **405**, 661 (2000); M.A. Baldo *et al.*, Nature **403**, 750 (2000); Y. Cao *et al.*, Nature **397**, 417 (1999); R.H. Friend *et al.*, Nature **397**, 121 (1999);

[2] L. Kilian, B. Cowie, J. Zegenhagen, P. Woodruff, private communication.

[3] F. Schreiber et al., Verhandl. DPG (VI) 36, 1 / SYOF 2.5 (2001)