



	Experiment title: SEXAFS and NIXSW on large organic molecular adsorbates on Ag(111)	Experiment number: SI-524
Beamline: ID 32	Date of experiment: from: 4.11.1999 to: 16.11.1999	Date of report: 18.2.2000
Shifts: 24	Local contact(s): B. Cowie	<i>Received at ESRF:</i>
Names and affiliations of applicants (* indicates experimentalists): L. Kilian*, Exp. Physik II, Univ. Würzburg, Am Hubland, D-97074 Würzburg, Germany M. Sokolowski*, Exp. Physik II, Univ. Würzburg, Am Hubland, D-97074 Würzburg, Germany H. L. Meyerheim*, Inst. f. Kristallographie, LMU München, Theresienstr.41, D-80333 München H. Maltor*, Inst. f. Kristallographie, LMU München, Theresienstr.41, D-80333 München B. Cowie*, ESRF, F-38043 Grenoble E. Umbach, Exp. Physik II, Univ. Würzburg, Am Hubland, D-97074 Würzburg, Germany		

Report: During the last years, the adsorption of large π -conjugated organic molecules containing several aromatic rings on surfaces has gained strong interest under fundamental and technological aspects [1]. One issue is the detailed description of the adsorption geometry, i.e. the analysis of the intermolecular and the intramolecular structure (which is often modified upon adsorption) as well as the specific adsorption site.

In the normal incidence x-ray standing wave experiment (NIXSW) we have investigated a monolayer of endcapped-quaterthiophene (EC4T). This molecule forms a commensurate superstructure on Ag(111) [2,3] and is an ideal candidate for detailed structural investigations. The superstructure was prepared by sublimation of EC4T onto the Ag(111) surface under UHV. XPS spectra of the S1s and Ag-MNN Auger intensities (EDCs) were recorded in the normal incidence x-ray standing wave field at photon energies usually between 2,616 to 2,624 eV. A typical normalised absorption profile of the (111) Bragg reflection is shown in Fig. 1.

From the S1s XPS spectra taken during the NIXSW experiment and additional C1s and S1s spectra taken with higher resolution and high statistics *no* indications for a chemical modification of the EC4T layer by the x-ray beam could be deduced.

The NIXSW data were fitted using the program written by Woodruff et al. [4]. The results are summarised in Tab. 1. The vertical height of the S above the Ag(111) bulk planes was determined as 3.25 ± 0.1 Å. The coherent fraction of the S is found to be considerably smaller than for Ag, which may indicate that the four S atoms within each molecule are adsorbed on different sites and/or that there exists some disorder in the superstructure. The coherent fraction of the S at the ($\bar{1}$ 11) Bragg reflection is of the same order as for the (111) Bragg reflection. This is so far not understood, since this would indicate that S atoms are situated on high symmetry adsorption sites, which is, however, controversial to the p2 symmetry of the lateral order in the superstructure (determined from SXRD).

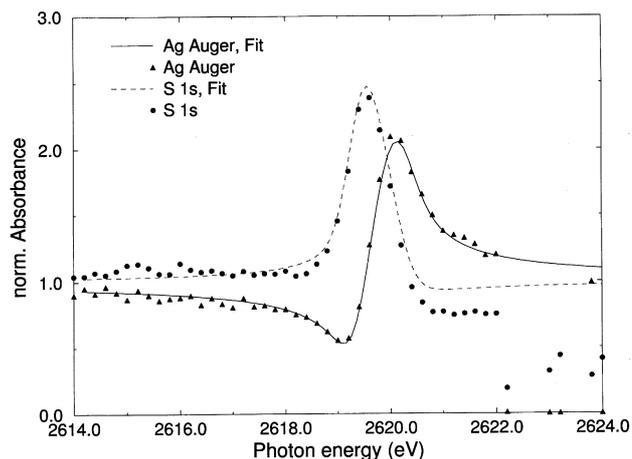


Fig. 1: Relative absorption versus photon energy recorded at the (111) Bragg reflection of an EC4T monolayer on Ag(111). Circles correspond to the Ag Auger intensity; triangles correspond to S1s photoemission intensity. The lines are the fits to the data.

The analysis of the NIXSW geometric fitting parameters in the frame of a structural model of the EC4T on Ag(111) which is compatible with the intermolecular structural parameters determined from SXRD [3] is still under progress. In addition, the quality of the fits to the NIXSW signal needs to be improved, e.g. the change of the intensity of the x-ray beam with time during the NIXSW run has to be taken into account. The determined geometric parameters are presently investigated in relation to the structural model obtained so far from LEED, STM and SXRD.

Absorber	(111) parameters		$(\bar{1}11)$ parameters	
	Spacing (\AA)	Coh. fract.	Spacing (\AA)	Coh. fract.
Ag	2.36	0.85	2.36	0.80
S	3.25	0.5	3.50	0.5

Tab. 1: Summary of layer spacings and coherent fractions obtained from fits to the experimental NIXSW data from EC4T/Ag(111).

References:

- [1] E. Umbach, M. Sokolowski, R. Fink. *Applied Physics A* **63** (1996) 565.
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- [3] H. L. Meyerheim, Th. Gloege, M. Sokolowski, E. Umbach, P. Bäuerle, *Phys. Rev. Lett.*, submitted.
- [4] B. Cowie, P. Woodruff, private communication.