

Surface X-ray Analysis of End-capped quinque Thiophene on Ag(111)

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Abstract No. malt1297

Beamline(s): X22C

Introduction: The structure of a large organic molecule [end-capped quinque-thiophene (EC5T)] was investigated by surface x-ray diffraction (SXRD). The structure formula is shown in Fig.1. Polythiophenes are model systems for light emitting diodes and have been intensively studied in the past by different methods such as by scanning tunneling microscopy and (STM) and low energy electron diffraction (LEED) [1], however, detailed structure analyses revealing the coordinates of the atoms within the unit cell have been carried out only recently for EC4T and uracil-derivatives [2].

Methods and Materials: EC5T was deposited on Ag (111) following the preparation outlined in Ref. [1].

Results: The reflection intensities are extremely weak, in total 10 independent in-plane reflections and 7 super-lattice rods were measured. The molecular superstructure was very stable during the experiments. On the Ag(111) surface, EC5T forms an incommensurate superstructure whose axes relative to the Ag(111)-(1x1) surface unit cell are described by the

matrix $\begin{pmatrix} 2.6394 & 1.1533 \\ 3.0624 & 18.8865 \end{pmatrix}$ (unit cell with parameters: $a_0 = 6.621\text{Å}$, $b_0 = 50.722\text{Å}$, $\gamma = 85.48^\circ$).

Conclusions: The Fig. 2 shows the z-projected Patterson-function calculated from the in-plane data. Apart from the maximum at the origin, there is one Patterson-peak at $y \approx 0.40$ along the b-axis corresponding to an inter-atomic vector of about 20 Å. It is labeled by "1". This peak can be related to correlation of thiophene rings between different molecules parallel to the b-axis. This strongly supports the "herringbone" model of the EC5T adlayer as developed in Ref. [1] on the basis of STM. Furthermore, from the rapid drop of the intensity along the superstructure rods the presence of some normal disorder can be inferred. The data analysis is still in progress.

Acknowledgments: H. Maltor and M. Gierer thank for the hospitality during their stay in Brookhaven and for providing access to beamline X22C. We also thank P. Bäuerle (University of Ulm) for providing EC5T. This work is supported by the SFB 338 of the DFG. Work at the NSLS is supported by the DOE.

References: [1] A. Soukopp, K. Glöckler, P. Kraft, S. Schmitt, M. Sokolowski, E. Umbach, E. Mena-Osteritz, P. Bäuerle, and E. Hädicke, Phys. Rev. **B 58**, 13882 (1998);

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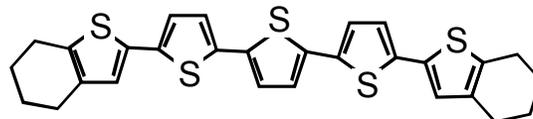


Figure 1. Structure formula of EC5T.

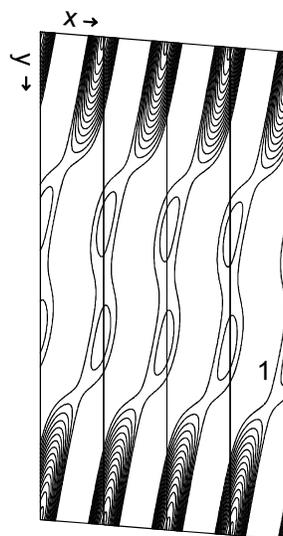


Figure 2. P(u,v) of EC5T/Ag(111). Four unit cells are shown.