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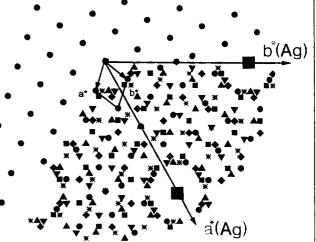
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Report: Using surface X-ray diffraction (SXRD) we proposed to investigate the geometric structure of large organic molecules which on Ag(111) form commensurate superstructures. As an example we have chosen End-Capped Quater-Thiophene (EC4T) which has been thoroughly investigated in the past [1,2]. From LEED and STM measurements it is known that EC4T forms a commensurate superstructure on Ag(111).

The figure 1 shows a schematically the reciprocal lattice of the system in projection along the c* axis.

Figure 1: Reciprocal lattice of EC4T/Ag(111): The solid parallelogram indicates the superstructure unit cell which in direct space is related to the Ag(111)-(1x1) surface unit cell by the matrix elements $a_{11}=2$, $a_{12}=-3$, $a_{21}=4$, $a_{22}=5$.

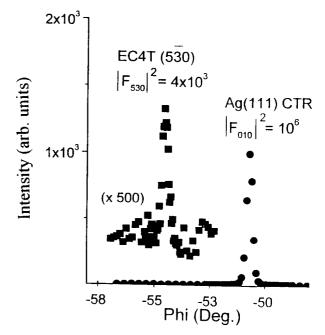


The large solid squares represent the first order Ag-reflections, all other symbols correspond to the superstructure, where each symbol type represents one of six equivalent domains. The unit cell of one domain is indicated by the solid parallelogram.

Due to the large unit cell, the weak scattering power of the atoms constituting organic molecules (24 C-atoms and 4 S atoms in the present case) and the low symmetry SXRD reflections are extremely weak.

The figure 2 compares the reflection profiles of the EC4T $(5\overline{3}0)$ reflection with the Ag(010) crystal truncation reflection, the intensity of the latter being equivalent with the scattering intensity of $^{1}/_{3}$ of a Ag monolayer.

Figure 2: Reflection profiles from EC4T and the Ag-crystal truncation rod. Note, that the EC4T profile is exaggerated by a factor 500.



Unfortunately, during the ESRF measurements it was not possible to prepare the superstructure with sufficient quality to allow the collection of a large data set. This problem has been solved meanwhile and the superstructures were prepared with high quality to allow the structure analysis [3].

References:

- [1] A Soukopp, K. Glöckler, P. Kraft, S. Schmitt, M. Sokolowski, E. Umbach, E. Mena.Osterlitz, P. Bäuerle, and E. Hädicke, Phys. Rev. B58, 13882 (1998)
- [2] C. Seidel, A. Soukopp, R. Li, P. Bäuerle, and E. Umbach, Surf. Sci. 374, 17 (1997)
- [3] H. L. Meyerheim, Th. Gloege, M. Sokolowski, E. Umbach, and P. Bäuerle, submitted for publication