



	Experiment title: In situ growth studies of sexiphenyl / sexithiophene heterostructures on TiO₂(110)	Experiment number: SI-1293
Beamline: BM 32	Date of experiment: from: 30. 11. 2005 to: 6.12. 2005	Date of report:
Shifts: 18	Local contact(s): Dr. Gilles Renaud	<i>Received at ESRF:</i>

Names and affiliations of applicants (* indicates experimentalists):

- * **Georg Koller**, Institute of Physics, KF-University Graz, Austria
- * **Martin Oehzelt**, Institute of Physics, KF-University Graz, Austria
- * **Thomas Haber**, Institute of Solid State Physics, Graz University of Technology, Austria
- * **Jan Ivanco**, Institute of Physics, University Graz, Austria
- Roland Resel**, Institute of Solid State Physics, Graz University of Technology, Austria
- Michael Ramsey**, Institute of Physics, University Graz, Austria
- Annette Thierry**, Institute Charles Sadron, Strasbourg, France

Report:

Sexiphenyl and Sexithiophene heterostructures grown on TiO₂ (110) and p(2x1)O reconstructed Cu (110) surfaces have been investigated. Major results are summarized in the following two papers, which have been accepted for publication.

Organic Heteroepitaxy: *Para*-sexiphenyl on Uniaxially Oriented α -sexithiophene

Adv. Mater. in press (2006):

M. Oehzelt^{a,b*}, G. Koller^a, J. Ivanco^a, S. Berkebile^a, T. Haber^b, R. Resel^b, F.P. Netzer^a, M.G. Ramsey^a

a, Institute of Physics, Karl-Franzens-University, A-8010 Graz (Austria)

b, Institute of Solid State Physics, Graz University of Technology, A-8010 Graz (Austria)

Thin films of organic molecules have attracted considerable interest as active elements for optoelectronic devices such as organic light emitting diodes (OLED), organic field effect transistors (OFET) and photovoltaic cells. *Para*-sexiphenyl (6P) was one of the first materials where an efficient blue OLED was built^[1,2] and α -sexithiophene (6T) is known to have high field effect mobility in OFETs.^[3,4] The majority of the device relevant properties depend crucially on the crystal quality of the organic films.^[5] Moreover, the optoelectronic properties are highly anisotropic and depend on the orientation of the molecules within these

films.^[6] Therefore it is highly desirable to obtain organic layers with high order and well defined orientation. As modern devices tend to have a multiplicity of different organic layers it is important to understand organic-organic heteroepitaxy. Up to now studies have tended to concentrate on the organic on inorganic growth,^[7] with only very few controlled investigations of the organic on organic growth.^[8,9] The present paper focuses on the organic-organic growth.

One way to achieve ordered growth of thin films is to deposit molecules on an ordered substrate which serves as a template. For example the growth of 6P on an Al(111) substrate, which has a three-fold symmetry at the surface, results in the growth of three equivalent domains within the film.^[10] Recently it was shown that a substrate with two-fold symmetry is a suitable template to obtain well oriented uniaxial organic films.^[11] These examples illustrate that the reduction of the symmetry of the substrate lowers the number of equivalent domains. In the present study we used Cu(110) with half a monolayer of adsorbed oxygen as a substrate, which forms a Cu (110) – p(2x1)O surface reconstruction and a surface with two-fold symmetry. This substrate is highly corrugated with the copper-oxygen rows equally spaced by 5.1 Å along the [001] direction of the Cu surface.^[12] These copper oxygen rows (Cu-O) will be used as the template for directing the molecular film growth. Here we report that all deposited 6T molecules on this surface are aligned parallel to the Cu-O rows. Subsequently, 6P molecules were deposited on top of the 6T layer and it is shown that the 6P molecules align predominantly with their long molecular axes parallel to the 6T molecules.

The epitaxial sexiphenyl(001) monolayer on TiO₂(110): a grazing incidence x-ray diffraction study

Surface Science in press (2006):

R. Resel ^{a,*}, M. Oehzelt ^{a,e}, O. Lengyel ^a, T. Haber ^a, T. U. Schüllli ^b, A. Thierry ^c,
G. Hlawacek ^{d,e}, C. Teichert ^d, S. Berkebile ^e, G. Koller ^e, M. G. Ramsey ^e

^a Institute of Solid State Physics, Graz University of Technology, Petersgasse 16, A-8010 Graz, Austria

^b CEA Grenoble, DRFMC/SP2M/NRS, 17 avenue des Martyrs, 38054 Grenoble, France

^c Institute Charles Sadron, CNRS-UPR 22, 6, rue Boussingault, Strasbourg, France

^d Institute of Physics, University Leoben, Franz Josef Straße 18, 8700 Leoben, Austria

^e Institute of Physics, Karl-Franzens University Graz, Universitätsplatz 5, 8010 Graz

A para-sexiphenyl monolayer of near up-right standing molecules (nominal thickness of 30Å) is investigated *in-situ* by x-ray diffraction using synchrotron radiation and *ex-situ* by atomic force microscopy. A terrace like morphology is observed, the step height between the terraces is approximately one molecular length. The monolayer terraces, larger than 20 µm in size, are extended along the [001] direction of the TiO₂(110) substrate i.e. along the Ti-O rows of the reconstructed substrate surface. The structure of the monolayer and its epitaxial relationship to the substrate is determined by grazing incidence x-ray diffraction. Extremely sharp diffraction peaks reveal high crystalline order within the monolayer, which was found to have the bulk structure of sexiphenyl. The monolayer terraces are epitaxially oriented with the (001) plane parallel to the substrate surface (out-of-plane order). Four epitaxial relationships are observed. This in-plane alignment is determined by the arrangement of the terminal phenyl rings of the sexiphenyl molecules parallel to the oxygen rows of the substrate.