O 20 Organische Dünnschichten II

Zeit: Samstag 10:45–13:00 Raum: TU EB202

O 20.1 Sa 10:45 TU EB202

Interface Formation of Phthalocyanines with Hydrogen Passivated Si(111) — •Mihaela Gorgoi and Dietrich R.T. Zahn — Institut für Physik, Technische Universität Chemnitz, D-09107 Chemnitz, Deutschland

Hybrid devices such as organic light emitting diodes, solar cells or thin film transistors, based on phthalocyanine (Pcs) materials and silicon receive special attention nowadays. Therefore the knowledge of the Pc/Si interface electronic properties is required. This work studies the interface formation between the organic semiconductors, namely copper phthalocyanine ($CuPc$) and perfluorinated copper phthalocyanines (F_4CuPc,$F_{16}CuPc$), and hydrogen passivated Si(111) using photoemission and inverse photoemission spectroscopy. With these techniques the energy level alignment of the highest occupied and lowest unoccupied molecular orbitals (HOMO and LUMO) with the valence band maximum (VBM) and the conduction band minimum (CBM) of Si are determined. The HOMO and LUMO for the three materials reveal dissimilar trends in the direction of energy shifts as a function of Pcs thickness. While for $CuPc$ the shift is towards higher binding energy with increasing film thickness, for $F_{16}CuPc$ both HOMO and LUMO are shifting towards lower binding energy. The energy shifts are proposed to originate from changes in molecular orientation and the direction of the shifts to arise from the degree of fluorination.

O 20.2 Sa 11:00 TU EB202

A simple model system for silicon/organic interfaces: Si(111)-CH_3 — •Ralf Hunger[1], Rainer Fritsche[1], Bengt Jaeckel[1], Taek Lim[1], Lauren J. Webb[2], Nathan S. Lewis[2], and Wolfram Jaegermann[1] — [1]Darmstadt University of Technology, Surface Science Division, Department of Materials Science, Petersenstr. 23, 64287 Darmstadt — [2]California Institute of Technology, Division of Chemistry and Chemical Engineering, Pasadena, CA 91125

Conceptually, methyl-terminated silicon (111), Si(111)-CH_3, is one of the simplest possible silicon-organic interface structures. The Si(111)-CH_3 structure may serve as a reference system for more complex silicon/organic interfaces. It has the inherent advantage that the silicon surface is chemically and electronically passivated by the methyl-termination.

Employing high resolution synchrotron and ultraviolet photoelectron spectroscopy and low energy electron diffraction, we have analyzed the properties of Si(111)-CH_3 surfaces that were prepared in a wet chemical two-step chlorination/alkylation process. The investigations show that well-defined surfaces with high chemical stability and near ideal electronic passivation could be obtained. A (1x1) surface structure, a well-defined carbon 1s core level emission, and in the Si2p line a distinct surface core level shift of the carbon-bonded surface silicon atoms are found. According to these results, methyl-terminated Si(111) appears as suitable template for the preparation of silicon/organic hybrid device structures.

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Growth of Alkylsiloxane monolayers on patterned silicon substrates — •Thorsten Balgar, Nils Hartmann, Steffen Franzka, and Eckart Hasselbrink — Universität Duisburg-Essen, Campus Essen, Fachbereich Chemie, Universitätsstr. 5, 45141 Essen

We present a laser direct writing technique for patterning of silicon substrates on the submicrometer scale. The patterned substrates are used for selective coating in a millimolar solution of Octadecyltrichlorosilane (OTS) [1]. The OTS molecules build up an alkylsiloxane monolayer via self-assembling in well defined surface areas [2][3]. Three different approaches were developed to create structured organic monolayers with lateral features ranging from several microns down to 120 nm.

[1] Th. Balgar, R. Bautista, N. Hartmann and E. Hasselbrink, Surf. Sci. 532-535 (2003) 963

[2] N. Hartmann, Th. Balgar, R. Bautista, S. Franzka and E. Hasselbrink, Proc. SPIE 5223 (2003) 9, Physical Chemistry of Interfaces and Nanomaterials II

[3] Th. Balgar, S. Franzka, N. Hartmann and E. Hasselbrink, Langmuir 20 (2004) 3525

O 20.4 Sa 11:30 TU EB202

Submicron chemical patterning of silicon substrates by laser direct writing: A simple photothermochemical model — •Nils Hartmann, Thorsten Balgar, Steffen Franzka, and Eckart Hasselbrink — Universität Duisburg-Essen, Campus Essen, Fachbereich Chemie, Universitätsstr. 5, 45141 Essen

Recently laser direct writing has been shown to provide a versatile means for the preparation of laterally structured alkylsiloxane monolayers on silicon substrates [1,2]. Respective procedures either are based on the preparation of suitable templates or on direct patterning of coated substrates. A common feature of all these procedures is the capability to create patterns with lateral dimensions which are significantly below the diffraction-limited laser spot diameter. At a $1/e^2$ laser spot diameter of 2.5 microns, for example, well-confined lines with a width down to 120 nanometers have been prepared. Here we present a simple model, which considers the laser-assisted local annealing of the substrate and the strongly temperature dependent kinetics of the initiated chemical processes. The model allows to reproduce the experimentally observed dependence of the line width on the incident laser power and the writing speed and provides a simple explanation for the unexpectedly high resolution capability of the patterning technique.

[1] Th. Balgar, S. Franzka, N. Hartmann and E. Hasselbrink, Langmuir 2004, 20, 3525.

[2] N. Hartmann, Th. Balgar, R. Bautista, D. Dahlhaus, S. Franzka and E. Hasselbrink, Proc. SPIE 2003, 5223, 9.

O 20.5 Sa 11:45 TU EB202

Engineering of GaAs (100) surface with 4'-substituted aromatic self-assembled monolayers — •Michael Zharnikov[1], Andrey Shaporenko[1], Adlkofer Klaus[2], Avi Ulman[3], Michael Grunze[1], and Motomu Tanaka[2] — [1]Angewandte Physikalische Chemie, Universität Heidelberg, Im Neuenheimer Feld 253, D-69120 Heidelberg, Germany — [2]Lehrstuhl für Biophysik E22, Technische Universität München, James-Franck-Strasse, D-85748, Garching, Germany — [3]Department of Chemical Engineering, Polytechnic University, Brooklyn 11201, New York, USA

High-resolution x-ray photoelectron spectroscopy and near edge x-ray absorption fine structure spectroscopy were applied to characterize GaAs (100) surface engineered by self-assembled monolayers (SAMs) of 4'-substituted aromatic molecules: 4'-methyl-4-mercaptobiphenyl (CH_3-BPT) and 4'-hydroxy-4-mercaptobiphenyl (OH-BPT). These molecules were found to form ordered and densely packed SAMs on GaAs, which were able to protect the substrate from degradation under ambient conditions. The molecular attachment in the SAMs occurs over As-thiolate bond while the intact aromatic backbones have an upright orientation with average tilt angles of 31.0° and 37.2° for CH_3-BPT and OH-BPT films, respectively. The difference in the tilt angle is attributed to a higher (by 7-10%) packing density of the former SAM, suggesting that the character of 4'-substitution affects the SAM quality in the case of GaAs substrate.

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In-Situ study of the first stages of F16CuPc growth on SiO2 — •Dimas Garcia de Oteyza [1], Esther Barrena[1], Oriol Ossó[2], Stefan Sellner[1], and Helmut Dosch[1,3] — [1]Max Planck Institut für Metallforschung, Stuttgart — [2]Institut de Ciència de Materials de Barcelona, CSIC — [3]Institut für Theoretische und Angewandte Physik, Universität Stuttgart

We have studied the first stages of F16CuPc growth on SiO2 by AFM and in-situ X-ray measurements. For thicker films they form a well ordered layered structure, with layers of virtually upright standing molecules and a spacing of 14.3 Å. At low coverage, both techniques coincide in the observation of striking structural changes on the first layers. The layer heights found for the first, second and third layers are 12.5 Å, 15 Å and 21 Å respectively. Besides, both the size and the aspect ratio of the elongated crystallites increase in the subsequent layers. From the X-ray data an additional layer at the interface with the SiO2 is obtained. This layer has a saturation thickness of around 6.5 Å and it shows a periodicity in the surface plane of 15 Å, which corresponds to the molecular size along one of its sides. The electronic density of this interfacial layer is about half of the electronic density of the thicker films. The growth behaviour of the first 3 layers has been characterized by both techniques. AFM and in-situ X-ray diffraction show a very good agreement.

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Strongly Enhanced Thermal Stability of Crystalline Organic Thin Films Induced by Aluminum Oxide Capping Layers — •S. Sellner[1,2], A. Gerlach[3], F. Schreiber[3], M. Kelsch[1], N. Kasper[1], H. Dosch[1,2], S. Meyer[4], J. Pflaum[4], M. Fischer[5], and B. Gompf[5] — [1]Max-Planck-Institut für Metallforschung, Stuttgart, Germany — [2]Institut für Theoretische und Angewandte Physik, Universität Stuttgart, Germany — [3]Physical and Theoretical Chemistry Laboratory, Oxford University, UK — [4]III. Physikalisches Institut, Universität Stuttgart, Germany — [5]I. Physikalisches Institut, Universität Stuttgart, Germany

We show that the thermal stability of organic semiconductor thin films can be strongly enhanced by capping with an aluminum oxide layer. By thermal desorption spectroscopy and *in-situ* X-ray diffraction we demonstrat that organic films do not only stay on the substrate, but even remain crystalline up to 270°C above their desorption point for uncapped films [1]. Different parameters contributing to the stability enhancement and eventual breakdown of the crystalline order of the organic film at elevated temperatures were identified. We argue that this very efficient enhancement of the thermal stability compared to uncapped and also to metal-capped organic layers is related to the low mobility of aluminum oxide and the structurally well-defined as-grown interfaces exhibiting limited interdiffusion. Possible mechanisms for the eventual breakdown at high temperatures will be discussed.

[1] Sellner et al., Adv. Mat. 16 (2004), p. 1750

O 20.8 Sa 12:30 TU EB202

Transport in capped organic thin film transistors at elevated temperatures — •S. Meyer[1], J. Wrachtrup[1], J. Pflaum[1], S. Sellner[2], G. Ulbricht[2], A. Gerlach[3], F. Schreiber[3], M. Fischer[4], and B. Gompf[4] — [1]III. Physikalisches Institut, Universität Stuttgart — [2]Max-Planck-Institut für Metallforschung, Stuttgart — [3]Physical and Theoretical Chemistry Laboratory, Oxford University, UK — [4]I. Physikalisches Institut, Universität Stuttgart

The thermal stability of the organic semiconducting layer is of crucial importance for the device performance in organic electronics. To address this problem we have performed comparative studies on organic thin film transistors (OTFTs) utilizing pentacene thin films with and without capping layer. The latter is realized by a 50nm thick sputter layer of aluminum oxide. On pentacene TFTs a field-effect is demonstrated up to temperatures of 250°C which is about 170°C above the desorption point of uncapped pentacene films on SiO_2. From the TFTs characteristics a complex behavior of the temperature dependent hole mobility and threshold voltage can be deduced, indicating that the device operation at these elevated temperatures is predominantly limited by the transistor structure, i.e. metal-diffusion at the contacts, and not by the organic material. Detailed studies by thermal desorption spectroscopy and X-ray diffraction on capped pentacene and diindenoperylene thin films show that the organic layer remains crystalline far above the breakdown temperature of the TFTs as a function of heating rate, thickness and stoichiometry of the AlOx. capping layer [1].

[1] Sellner et al., Adv. Mat. **16** (2004) 1750

O 20.9 Sa 12:45 TU EB202

Post-functionalization of self-assembled alkylsiloxane monolayers for gold colloid adsorption — •Daniel Dahlhaus, Steffen Franzka, Nils Hartmann, and Eckart Hasselbrink — Universität Duisburg-Essen, Campus Essen, Fachbereich Chemie, Universitätsstr. 5, 45141 Essen

Self-assembled monolayers (SAMs) are widely recognized for their use in a range of technological applications, including optoelectronic devices and biological sensors. Depending on the detailed application SAMs with varying terminal groups are required. Of particular interest for the adsorption of gold nanoparticles are SAMs exposing amino and thiol groups. In our experiments we first prepared octadecylsiloxane (ODS) monolayers by immersion of freshly cleaned silicon oxide substrates in a millimolar solution of octadecyltrichlorosilane [1]. For characterization contact angle measurements and atomic force microscopy were used. A chemical functionalization of the ODS monolayers has then been achieved by free-radical bromination using visible light. Subsequently, the bromine groups can be replaced by other functional groups such as amines and thiols [2]. Preliminary results indicate the adsorption of gold colloids on these functionalized ODS monolayers.

[1] N. Hartmann, T. Balgar, R. Bautista, E. Hasselbrink, Surf. Sci., 532-535 (2003) 963.

[2] N. Balachander, C.N. Sukenik, Langmuir, 6 (1990) 1621.