

DS 22: Organic Thin Films II

Time: Wednesday 11:15–13:00

Location: GER 38

DS 22.1 Wed 11:15 GER 38

Real-time detection of optical changes of diindenoperylene thin films during growth — •UTE HEINEMEYER¹, REINHARD SCHOLZ², ALEXANDER GERLACH¹, and FRANK SCHREIBER¹ — ¹Institut für Angewandte Physik, Auf der Morgenstelle 10, 72076 Tübingen — ²Walter Schottky Institut, Technische Universität München, Am Coulombwall 3, 85748 Garching

Organic semiconductors have attracted increasing interest, mainly due to their potential optoelectronic applications like organic light emitting diodes and organic solar cells. Optimization of device performance requires the understanding of the underlying structure and growth behavior. Therefore, real-time measurements are particularly powerful since they detect possible changes in the functional properties already during growth. Diindenoperylene (DIP) shows a particularly well defined ordering and promising electronic transport properties together with a highly anisotropic dielectric function [1]. Differential reflectance spectroscopy (DRS), a non-invasive optical technique with high sensitivity, is used to follow the film growth of DIP on glass in the spectral range between 1.4 eV and 3.1 eV. The optical spectra show the well known vibronic progression together with an additional transition, which is related to the coupling between the molecules. The real-time growth experiments show how this additional transition arises during growth, indicating that the intermolecular coupling changes with increasing film thickness, whereas the vibronic progression is only slightly changed.

[1] U. Heinemeyer, R. Scholz *et al.*, PRB **78**, 085210 (2008)

DS 22.2 Wed 11:30 GER 38

In-situ optical spectroscopy of ultrathin quaterylene films epitaxially grown on graphite and mica — •ROMAN FORKER, CHRISTIAN GOLNIK, CHRISTIAN WAGNER, MORITZ ESSLINGER, and TORSTEN FRITZ — Institut für Angewandte Photophysik, Technische Universität Dresden, 01062 Dresden, Germany

Profound knowledge of the growth behavior of aromatic molecules on insulating and conducting substrates is highly desired since an alignment of the planar π -electron cores in face-on or edge-on geometry, respectively, will have a direct impact on the performance of devices, such as solar cells or OFETs. Here we report the epitaxial growth of quaterylene (QT, C₄₀H₂₀) deposited on single-crystalline graphite and mica, as examined *in-situ* by a variant of optical absorption spectroscopy, namely differential reflectance spectroscopy (DRS). We found substantial differences in the shape and in the film-thickness-dependent evolution of the spectra that can only be understood in terms of dissimilar growth modes on these substrates. While the optical behavior of QT films on graphite resembles that of QT reported for a face-on heteroepitaxial arrangement on Au(111) [1], the growth of QT films on mica can more likely be described by an edge-on assembly, as also observed on SiO₂ [2]. With the help of low-energy electron diffraction (LEED) measurements we can evidence the occurrence of flat-lying QT molecules on graphite. In turn, we can exclude such a growth mode on mica, due to the fundamentally different optical spectra in that case. [1] R. Forker *et al.*, Adv. Mater. *in press*, 10.1002/adma.200801112. [2] R. Hayakawa *et al.*, J. Phys. Chem. C **111** (2007), 18703.

DS 22.3 Wed 11:45 GER 38

Crystalline to semi-crystalline phase transitions in thin *n*-Dotriacontane films on solid surfaces — EDGARDO A. CISTERNAS¹, TOMÁS CORRALES¹, VALERIA DEL CAMPO¹, •ULRICH G. VOLKMANN¹, HASKELL TAUB², and FLEMMING Y. HANSEN³ — ¹Surface Lab, Facultad de Física, Pontificia Universidad Católica de Chile, Chile — ²Department of Physics and Astronomy, University of Missouri-Columbia, USA — ³Department of Chemistry, Technical University of Denmark, Denmark.

We present evidence from ellipsometric measurements of crystalline to semi-crystalline or rotator transitions on molecularly thin films of the intermediate length alkane *n*-Dotriacontane (*n*-C₃₂H₆₆), grown on Si(100) substrates covered with their native oxide layer. We are able to grow films with three different morphologies: 1) submonolayer coverage with the molecules perpendicular to the surface, 2) multilayered films with high coverage of the first perpendicular layer without bulk and 3) multilayered films with bulk particles. For submonolayer coverage films we found one step in the ellipsometer signal at ~331 K which

can be correlated to a rotator phase transition. For multilayered films we observe additional steps in the ellipsometric signal which are correlated to changes in upper molecular layers and to rotator phases in bulk crystallites, respectively. A theoretical interpretation of the ellipsometric data is presented to explain these steps in the signal as changes in the anisotropy of the polarizability tensor of the alkane molecules.

DS 22.4 Wed 12:00 GER 38

Optical modelling of organic light emitting diodes — •MAURO FURNO, ROBERT NITSCHKE, RICO MEERHEIM, BJÖRN LÜSSEM, and KARL LEO — Institut für Angewandte Photophysik, Technische Universität Dresden, George-Bähr-Straße 1, 01062 Dresden, Germany

The general structure of an organic light emitting diode (OLED) consists of various organic and metallic layers with different functionalities [1]. Since the complexity of the device structures is rapidly increasing, optical models are more and more required for the effective design and optimization of OLEDs. We present in this contribution a numeric optical model suitable for planar OLED structures. The model exploits the well-established equivalence between light emission from electrical dipole transitions and radiation from mutually-incoherent classical electromagnetic antennas, and a transfer matrix description of the OLED coherent multilayered structure [2]. To validate model results, we fabricated and electrically and optically characterized small-molecule p-i-n type OLED [3]. The whole of angularly and spectrally resolved radiometric and photometric intensities, as well as current, power and quantum efficiencies, and CIE coordinates are fitted by calculation results exploiting consistent parameters for devices with different structural features. Due to the excellent overall agreement between measurements and calculations, we generalize the model results and provide design guidelines for optically optimized OLEDs.

[1] K. Walzer *et al.*, Chem. Rev. **107**, 1233 (2007)

[2] H. Benisty *et al.*, J. Opt. Soc. Am. A **15**, 1192 (1998)

[3] R. Meerheim *et al.* Appl. Phys. Lett. **93**, 043310 (2008)

DS 22.5 Wed 12:15 GER 38

Effects of annealing and UV irradiation on pulsed laser deposited PMMA films — •BRITTA LENA FUCHS, ANDREAS MESCHEDER, and HANS-ULRICH KREBS — Institut für Materialphysik, Universität Göttingen, Friedrich-Hund-Platz 1, D-37077 Göttingen

Smooth thin films of Poly(methylmethacrylate) (PMMA) are of interest as photoresist or for coating applications. Here pulsed laser deposition (PLD) at a wavelength of 248 nm is used at low laser fluences slightly above the deposition threshold of PMMA (between 80 and 160 mJ cm⁻²) to prepare completely smooth films free of droplets [1]. The chemical behaviours were measured by infrared spectroscopy (FTIR) and size exclusion chromatography (SEC). By indentation measurements we find that these films are very soft after preparation and possess a universal hardness of only HU=5 N mm⁻². But after UV irradiation a strong hardening of the PMMA films occurs due to a higher cross-linking of the polymer. When depositing the PMMA films at higher substrate temperatures, we also observe a hardening of the films (above 200 N mm⁻²). But additionally a strong dewetting from the substrates occurs. Above 250 °C partial evaporation of the polymer becomes observable and the FTIR spectra do not show the characteristic vibration bands any more.

[1] B. Lösekrug, A. Meschede, H.U. Krebs, Appl. Surf. Sci. **254** (2007) 1312

DS 22.6 Wed 12:30 GER 38

Hierarchy of adhesion forces in patterns of photoreactive surface layers — •QUAN SHEN¹, NURDOGAN GÜRKAN¹, GREGOR HLAWACEK¹, CHRISTIAN TEICHERT¹, ALEXANDRA LEX², GREGOR TRIMMEL², and WOLFGANG KERN³ — ¹Institute of Physics, University of Leoben, 8700 Leoben, Austria — ²Institute of Chemistry and Technology of Organic Materials, Graz University of Technology, 8010 Graz, Austria — ³Institute of Chemistry of Polymeric Materials, University of Leoben, 8700 Leoben, Austria

In this contribution we focus on the investigation of ultrathin layers of the new photosensitive molecule trimethoxy[4-(thiocyanatomethyl)phenyl] silane. The photosensitive tail group, benzyl thiocyanate, undergoes a photoisomerization to the corresponding

isothiocyanate upon illumination with UV light. The illuminated regions can now react with amines to give regions with modified surface properties.

By illumination through a contact mask and subsequent modification, photochemically patterned surfaces are achieved [1]. Friction Force Microscopy (FFM) is used to distinguish between the chemically different areas in the pattern. Indeed, a significant friction contrast between up to four different tail groups is observed simultaneously on the same sample [2].

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[1] A. Lex, et al., Chem. Mater. 20, 2009-2015 (2008).

[2] G. Hlawacek, et al., arXiv:0810.2625v1 [cond-mat.mtrl-sci].

DS 22.7 Wed 12:45 GER 38

Chemical and electronic properties of the In-on-CuPc contact: a photoemission study — •TEODOR TOADER¹, JAN IVANCO¹, ALEXANDER FIRSOV², WALTER BRAUN², and D.R.T. ZAHN¹ — ¹Semiconductor Physics, Chemnitz University of Technology, D-09107 Chemnitz, Germany — ²BESSY GmbH, Albert-Einstein-Straße 15,

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The interfacial chemistry and the evolution of electronic structure was studied during the formation of a top indium contact on CuPc in ultra-high vacuum. The In 4d core level revealed two components: the metallic component and a second one shifted towards higher binding energy. In recent studies, such a shifted component was associated with the formation of a reactive In/CuPc interface. The appearance of so-called gap states near the Fermi level would also provide an argument in favor of a reactive interface. However, probing the interface at different photon energies revealed that the origin of the shifted component is located at the surface of In rather than buried at the In/CuPc interface, as one would expect for reactive components. Given also the fact that the other core levels C 1s and N 1s indicated no reaction between In and CuPc, we assume that both the shifted component in the In 4d core level and the gap states are due to final state effects and/or charging related to the formation of metallic nanoclusters instead of a continuous metallic film. The presence of indium nanoclusters on the CuPc surface is corroborated by the secondary electron microscopy (SEM).