

sient local temperature rise and the thermally activated desorption of the thiol molecules. A simple thermokinetic analysis of the data allows to estimate effective kinetic parameters of the patterning process. Respective values are in good agreement with data in the literature.

1. D. Dahlhaus, S. Franzka, E. Hasselbrink, N. Hartmann, Nano Lett. 6 (2006) 2358.

2. N. Hartmann, S. Franzka, J. Koch, B. N. Chichkov, A. Ostendorf, Appl. Phys. Lett. 92 (2008) 223111.

O 66.3 Fri 11:45 SCH A316

Laser-assisted chemical lithography via local photothermal functionalization of silane-based organic monolayers — ●BENJAMIN KLINGEBIEL, ANJA SCHRÖTER, and NILS HARTMANN — Fachbereich Chemie, Universität Duisburg-Essen (UDE) and Center for Nanointegration Duisburg-Essen (CeNIDE), Universitätsstraße 5, 45117 Essen

Photochemical routines are widely recognized as a versatile means to fabricate multifunctional patterned organic monolayers with laterally alternating chemical terminations. The lateral resolution, in turn, usually is limited to the micrometer and submicrometer length scales. A simple routine for nanopatterning of organic monolayers down to 100 nm and below relies on photothermal processes [1, 2]. For this purpose a focused laser beam is used to locally heat the substrate and initiate thermal decomposition of the monolayer. Here we report on a simple photothermal procedure for direct functionalization of organic monolayers. Surface-oxidized silicon samples are coated with alkylsiloxane monolayers. Local irradiation with a focused beam of an argon ion laser at a wavelength of 514 nm in gaseous bromine allows for direct functionalization of the monolayer. Mechanistic aspects and prospects of photothermal routines in micro- and nanofabrication of multifunctional organic monolayers are discussed.

1. D. Dahlhaus, S. Franzka, E. Hasselbrink, N. Hartmann, Nano Lett. 6 (2006) 2358.

2. N. Hartmann, B. Klingebiel, T. Balgar, S. Franzka, E. Hasselbrink, Appl. Phys. A 94 (2009) 95.

O 66.4 Fri 12:00 SCH A316

Infrared spectroscopic ellipsometry for characterization of functionalized thin films — ●D.M. ROSU¹, G. SUN¹, X. ZHANG², J. RAPPICH², J. JONES³, J.W.P. HSU³, U. SCHADE⁴, N. ESSER¹, and K. HINRICHS¹ — ¹Institute for Analytical Sciences, Albert-Einstein-Str. 9, 12489 Berlin, Germany — ²Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Kekuléstraße 5, 12489 Berlin, Germany — ³Sandia National Laboratories, Albuquerque, New Mexico 87185-1120 — ⁴Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Albert-Einstein-Str. 15, 12489 Berlin, Germany

Organic thin films present a high interest due to their potential use in a large variety of applications: biosensors, microelectronic and optical devices. In the current work Infrared Spectroscopic Ellipsometry was used for chemical and structural characterisation of bifunctional surfaces as well as for investigation of the lateral homogeneity of organic monolayers for GaAs hybrid diodes[1]. The samples were studied using a lab FTIR ellipsometer and the FTIR synchrotron mapping ellipsometer located at the IR beamline at BESSY II[2]. The mapping system enables investigation of heterogeneous samples with monolayer

sensitivity and a lateral resolution below 1 mm². Besides the molecular identification, evaluation of the measured spectra with simulations using optical layer models gives informations about thickness, homogeneity and orientation of the molecules.

[1] D.M. Rosu, et al., Langmuir, in print [2] M. Gensch, et al., Infrared Phys. and Techn. 49 (1-2) (2006) 39-44

O 66.5 Fri 12:15 SCH A316

Magnetron sputtered hydrogenated (a-C:H) and oxygen containing (a-C:O) amorphous carbon coatings: surface characteristics, wettability and cell absorption behaviour — ●FRIEDERIKE DANNEIL — Forschungszentrum Karlsruhe, Institut für Materialforschung I, Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen, Germany

Hydrogenated amorphous carbon (a-C:H) coatings are considered good potential materials for biomedical applications. Hydrogen-free, oxygen containing amorphous carbon (a-C:O) coatings exhibit promising haemocompatible properties but have not yet been investigated very detailed. The objective of this work is the characterization of the surface characteristics, surface properties, wettability and haemocompatibility both of a-C:H and a-C:O coatings prepared by reactive d.c. magnetron sputtering.

The coatings were deposited on Si wafer substrates by sputtering a graphite target in a mixture of methane and argon (Ar+CH₄) and a mixture of oxygen and argon (Ar+O₂), respectively. The reactive gas fractions were systematically varied during the experiments. For the surface characterization atomic force microscopy (AFM), Raman spectroscopy and X-ray photoelectron spectroscopy (XPS) were applied. The surface free energy was determined by contact angle measurements. A platelet adhesion test showed favourable behaviour of the a-C:O coatings for blood-contacting applications.

O 66.6 Fri 12:30 SCH A316

Microscopic and fluorescence spectroscopic studies of organic molecules in contact to surfaces — ●HEINRICH SÜDMEYER¹, FRANZ-JOSEF SCHMITT¹, JOACHIM BÖRNER¹, MAX SCHOENGEN¹, HANS-JOACHIM CAPPUS², and HANS JOACHIM EICHLER¹ — ¹Institut für Optik und Atomare Physik, Technische Universität Berlin, Strasse des 17. Juni 135, 10623 Berlin — ²Laser- und Medizin-Technologie GmbH, Fabekstrasse 60 - 62, 14195 Berlin

Specific amino acids contained in proteins show autofluorescence if excited in UV. Therefore the use of fluorescence markers is not necessary for high resolved fluorescence microscopy. On the other hand it is often necessary to immobilize proteins. But the photophysical and biochemical properties of organic molecules change due to surface contact. To understand these properties the change of protein conformations due to the surface contact must be analyzed. Combined microscopic and time correlated single photon counting methods (TCSPC) are very promising because the fluorescence depends on the conformational structure of the proteins and allows to analyze different quenching mechanisms. With TCSPC energy transfer processes between neighbouring amino acids, neighbouring molecules and between molecules and the surface can be analyzed. Due to the fluorescence kinetics it is also possible to separate the fluorescence of spectrally similar fluorescence emitters.

O 67: Ab-initio approaches to excitations in condensed matter III

Time: Friday 11:15–12:45

Location: SCH 251

O 67.1 Fri 11:15 SCH 251

Tackling localized *d*-states: a systematic investigation by $GW@LDA+U$ — ●HONG JIANG¹, RICARDO I. GOMEZ-ABAL¹, PATRICK RINKE^{2,1}, and MATTHIAS SCHEFFLER^{1,2} — ¹Fritz-Haber-Institut der MPG, Berlin — ²University of California at Santa Barbara, CA 93106

First-principles modeling of systems with localized *d*-states is currently a great challenge in condensed matter physics. Density-functional theory (DFT) in the standard local-density approximation (LDA) proves to be problematic. This can be partly overcome by including local Hubbard *U* corrections (LDA+*U*), but itinerant states are still treated on the LDA level. Many-body perturbation theory in the *GW* approach offers both a quasiparticle perspective (appropriate for itinerant states) and an exact treatment of exchange (appropriate for lo-

calized states), and is therefore promising for these systems. Here we present a systematic investigation of the G_0W_0 method based on LDA+*U* ($G_0W_0@LDA+U$) for a series of prototype systems: 1) ZnS with semicore *d*-states, 2) ScN and TiO₂ with empty *d*-states and 3) late transition metal oxides (MnO, FeO, CoO and NiO) with partially occupied *d*-states. We show that for ZnS, ScN and TiO₂, the G_0W_0 band gap only weakly depends on *U*, but for the other transition metal oxides the dependence on *U* is as strong as in LDA+*U*. These different trends can be understood in terms of changes in the hybridization and screening. Our work demonstrates that $G_0W_0@LDA+U$ with “physical” values of *U* provides a balanced and accurate description of both localized and itinerant states.

O 67.2 Fri 11:30 SCH 251

Spin-wave excitations in itinerant ferromagnets from