DS 42: Poster I: Progress in Micro- and Nanopatterning: Techniques and Applications (jointly with O); Spins in Organic Materials; Ion Interactions with Nano Scale Materials; Organic Electronics and Photovoltaics; Plasmonics and Nanophotonics (jointly with HL and O); High-k and Low-k Dielectrics (jointly with DF); Organic Thin Films; Nanoengineered Thin Films; Layer Deposition Processes; Layer Properties: Electrical, Optical, and Mechanical Properties; Thin Film Characterisation: Structure Analysis and Composition; Application of Thin Films

Time: Wednesday 15:00–17:30 Location: P1

DS 42.1 Wed 15:00 P1

Self-organized surface patterns on Si by sputter erosion with molybdenum surfactants — Kun Zhang, •Andre Pape, Marc Brötzmann, and Hans Hofsäss — II. Physikalisches Institut, Universität Göttingen,37077 Göttingen, Germany

We report on the self-organized pattern formation on Si surfaces driven by Mo surfactant atoms. Si substrates were irradiated with 5 keV Xe ions at normal and near normal ion incidence and fluences up to $5x10^{17}$ Xe^+/cm^2 under continuous deposition of Mo surfactant atoms. In the absence of Mo deposition uniform flat surfaces are obtained. With Mo surfactants pronounced patterns like dots, combinations of dots and ripples as well as ripples with about 100 nm wavelength and up to 12 nm in height are generated. The patterns are analyzed with atomic force microscopy, Rutherford backscattering and transmission electron microscopy. We analyze the critical Mo steady-state coverage for onset of dot formation and onset of ripple formation and the evolution of the pattern contrast with increasing ion fluence. Pattern formation is explained by ion induced diffusion and phase separation of an initially flat amorphous Mo_xSi layer and subsequent ion beam erosion with composition dependent sputter yield. Directed deposition of Mo causes preferential deposition and shadowing and determines the final pattern orientation and morphology.

DS 42.2 Wed 15:00 P1

Functionalization of oxide and oxide-metallic nanowire arrays — •Anshuma Pathak[1,2], Hongdan Yan[1], Johannes Dühn[1], Mehmet Fatih Cetin[1], Meinhard Schilling[3], Marc Tornow[2], and Peter Lemmens[1] — [1]IPKM, TU-BS, Braunschweig, Germany — [2]IHT, TU-BS, Braunschweig, Germany — [3]EMG, TU-BS, Braunschweig, Germany

We investigate the functionalization of single crystalline, nanocrystalline and nanoporous Al_2O_3 surfaces as a coupling enabler to different molecular species. Our aim is to establish nanostructured, composite oxide-molecular materials that can be used as model systems for optically induced energy transfer. Nanoporous oxides are prepared using electrochemical oxidation leading to a dense array of pores. The pore walls are functionalized and in a subsequent step filled by Au wires using electrochemical deposition techniques. The characteristic length scales of the arrays are 20-30 nm with respect to diameter and distance of the pores. Specifically, we investigate the impact of different organic monolayer coatings to the pore walls on the growth and morphology of the Au nanowires.

Work supported by IGSM and NTH.

DS 42.3 Wed 15:00 P1

Surfactant assisted ion beam erosion of GaN and AlN surfaces — •Kun Zhang[1], Ulrich Vetter[1], Nils Borth[1], Hans-Gregor Gehrke[1], Ramasamy Jayavel[2], and Hans Hofsäss[1] — [1]II. Physikalisches Institut, Universität Göttingen, 37077 Göttingen, Germany — [2]Centre for Nanoscience and Technology, Anna University Chennai, 600025 India

We investigate the evolution of the surface morphology of AlN and GaN surfaces during ion beam erosion. AlN and GaN films grown on sapphire substrates were irradiated at room temperature with few keV Xe ions at normal ion incidence with ion fluences up to $4*10^{17}$ cm^{-2}. The surface morphology was analyzed using atomic force microscopy and scanning electron microscopy. For GaN selective sputtering causes segregation of Ga on the surface, resulting in a dense coverage with small spherical Ga droplets. With increasing ion fluence the droplet size increases. The Ga coverage was quantitatively analyzed with SEM and Rutherford backscattering. For AlN, the rms roughness of the surface decreases with increasing ion fluence from initially 8 nm to about 3 nm at $4*x10^{17}$ cm^{-2}. No ripple or dot patterns were observed. Sputtering of AlN with simultaneous co-deposition of Ga, results in the formation of randomly distributed small Ga droplets and $Al_{0.8}Ga_{0.2}$ islands of few nm in size on the AlN surface. The rms roughness of such a surface is only about 1.3 nm. The density of droplets and islands decreases with increasing ion fluence. In the intermediate regions the AlN surface appears rather flat with rms roughness well below 1 nm.

DS 42.4 Wed 15:00 P1

Selective surface modification of silicon oxide by OTS — •Christian Belgardt[1], Thomas Baumgärtel[1], Thomas Blaudeck[2], Harald Graaf[1], Reinhard R. Baumann[2], and Christian von Borczyskowski[1] — [1]Center for Nanostructured Materials and Analytics (nanoMA), Institute of Physics, Chemnitz University of Technology, 09107 Chemnitz, Germany — [2]Institute for Print and Media Technology (pmTUC), Chemnitz University of Technology, 09107 Chemnitz, Germany

The key material of electronics is silicon oxide. The chemical modification of its surfaces by self-assembled monolayers (SAMs) is a well-known method to control their physico-chemical properties. SAMs are typically formed by chemical reaction of the constituting molecules with the surface. The common process to prepare highly ordered monolayers is a chemical bath of a silane solution e.g. octadecyltrichlorosilane (OTS).

We report on hydrophobic OTS monolayers formed by standard method from chemical bath and by ink-jet printing which is known as a purely additive dynamic method and scalable technology. Our results indicate that a structured hydrophobization of the silicon oxide surface by inkjet printing is possible using OTS diluted in toluene at millimolar concentrations. The SAM formation is seems to be governed by an evaporation-driven self-assembly of the OTS molecules on the surface.

DS 42.5 Wed 15:00 P1

Influence of process and system parameters on the local oxidation of alkyl-terminated silicon — •Thomas Baumgärtel, Harald Graaf, and Christian von Borczyskowski — Center for Nanostructured Materials and Analytics, Institut für Physik, TU Chemnitz, 09107 Chemnitz, Germany

The local anodic oxidation (LAO) of silicon substrates by an atomic force microscope (AFM) is an electrochemical process which is influenced by multiple parameters. These can be divided into two major groups: system parameters and process parameters. Process parameters such as oxidation voltage, duration and ambient humidity can be tuned over a wide range of values during the experiment. System parameters on the other hand depend on equipment and materials themselves and are only difficult to control e.g. AFM tip shape, substrate conductivity and surface hydrophobicity. We investigated the influence of these parameters on the LAO process of silicon which is passivated by a self-assembled alkyl monolayer. Such monolayers are not only characterized by high molecular order and an excellent physical and chemical stability but offer also a neat way to tune the surface properties by variation of the head groups of the alkenes. A detailed understanding of the dependencies of the LAO process is essential for the controlled generation of silicon oxide nanostructures which can be used to build up functional nanostructures by a combined bottom-up (anchoring of functional molecules) and top-down (AFM LAO lithography) approach.

DS 42.6 Wed 15:00 P1

Permanent bending and alignment of ZnO nanowires — •Christian Borschel[1], Susann Spindler[1], Damiana Lerose[2,3], Arne Bochmann[3], Silke H. Christiansen[3,4], Sandor Nietzsche[5], Michael Oertel[1], and Carsten Ronning[1] — [1]Institut für Festkörperphysik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena — [2]MPI für Mikrostrukturphysik, Weinberg 2, 06120 Halle (Saale) — [3]Institut für Photonische Technologien, Albert-Einstein-Strasse 9, 07745 Jena — [4]MPI für die

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Ion beams can be used to bend or re-align nanowires permanently, after they have been grown. We have irradiated ZnO nanowires with ions of different species and energy, achieving bending and alignment in various directions. We study the bending of single nanowires as well as the simultaneous alignment of large ensembles of ZnO nanowires in detail. Computer simulations show that the bending is initiated by ion beam induced damage. Dislocations are identified to relax stresses and make the bending and alignment permanent and resistant against annealing procedures.

DS 42.7 Wed 15:00 P1

Investigation of conducting nanostructures on ta-C films made by FIB lithography — •Peter Philipp and Lothar Bischoff — Institute of Ion Beam Physics and Materials Research, Helmholtzzentrum Dresden-Rossendorf, P.O. Box 51 01 19, 01314 Dresden, Germany

Tetrahedral amorphous carbon (ta-C) films with high sp^3 content produced by mass filtered vacuum arc deposition were modified by Ga^+ FIB irradiation. Surface swelling occurs as a function of fluence, caused by ion induced conversion of sp^3 to sp^2 hybridized carbon atoms. A model [1] for diamond swelling was applied to ta-C films to estimate the swelling for fluences up to 1 x 10^{16} cm^{-2}. For higher fluences data from TRIDYN simulations were included due to sputtering in a good agreement with the experiments. Van der Pauw structures were produced by means of Ga^+ FIB lithography. A decrease of the sheet resistance with increasing fluence due to the evolution of graphitic regions was observed. The lowest value of 290 $\Omega/\Box$ was achieved at 1.6 x 10^{17} cm^{-2}. Additionally, conducting graphitic wires were produced (length: 10 μm, width: 300 nm to 5 μm). The wire resistivity was measured within 130 kΩ (5 μm width) and 0.3 GΩ (300 nm width). Ion induced graphitization of ta-C films by FIB offers prospective applications in nano technology to fabricate conductive nanostructures in an insulating thin film. [1] F. Bosia et al. Nucl. Instrum. Meth. B 268 (2010) 2991.

DS 42.8 Wed 15:00 P1

investigation of the depth profile of ion beam induced nanopatterns on Si with simultaneous metal incorporation — •Behnam Khanbabaee[1], Bahia Arezki[1], Andreas Biermanns[1], Marina Cornejo[2], Frank Frost[2], and Ullrich Pietsch[1] — [1]Festkörperphysik, Universität Siegen, Siegen, Germany — [2]Leibniz-Institut für Oberflächenmodifizierung (IOM), Leipzig, Germany

Ion beam sputtering of semiconductor surfaces can modify the surface and produce a diversity of surface topographies such as periodic ripples or dot structures depended on sputtering parameters. Well ordered nanostructured surfaces have widely technological applications. Recent experiments have shown that the incorporation of metallic impurity atoms during the sputtering process plays a crucial role in pattern formation on the surfaces. These findings offer a new degree of freedom to control pattern formation. In this contribution we report on surface patterning due to Kr ion beam erosion on silicon surfaces with simultaneous Fe and Cr incorporation. We used X-ray reflectivity (XRR) to determine the depth profiles of metal ions as function of ion beam divergence angles and the mean incidence angle of the ions with respect to the surface normal. Depth profiles are correlated with degree of pattern formation determined by AFM. We show that the mean penetration depth and concentration of metal ions depends on the divergence angle of Kr beam provided by Kaufman source which supports the assumption that metal ions are created due to parasitic interaction of the Kr beam with the steel plate lining. The evaluated depth profile by XRR is in good agreement with SIMS and RBS results.

DS 42.9 Wed 15:00 P1

Freestanding Si nanowires fabricated by Ga^+ FIB implantation and subsequent anisotropic etching — •Roman Böttger[1], Lothar Bischoff[1], Bernd Schmidt[1], and Matthias Krause[1,2] — [1]Helmholtzzentrum Dresden-Rossendorf, Institute of Ion Beam Physics and Materials Research, POB 510119, 01314 Dresden, Germany — [2]Technische Universität Dresden, Institut für Festkörperphysik, Zellescher Weg 16, 01062 Dresden, Germany

Localized Ga^+ ion implantation in silicon-on-insulator substrates (top layer 2 μm) by focused ion beam and subsequent anisotropic and selective wet etching has been used to fabricate freely suspended nanowires with reproducible widths between 20 and 200 nm. The dependence of the resulting nanowire width on the implanted fluence has been investigated and is supported by a numerical model reproducing the experimental data and enabling an a priori estimation of the nanowire width as a function of the implanted fluence. Moreover, the temperature dependence of the nanowires resistivity and the activation energy for electrical current flow were investigated before and after direct current annealing in air and in vacuum ambient. Annealed nanowires showed a decrease of their resistivity up to two orders of magnitude, indicating a partial recrystallization of the nanowires through self-heating and a change in the conduction mechanism. The assumption of recrystallization is supported by scanning electron microscopy and Raman spectroscopy. The comprehension of the pinpointed fabrication of such Si nanostructures establishes a broad range of application in the field of nano-electro-mechanical systems.

DS 42.10 Wed 15:00 P1

Nano Structure Formation on the Surfaces of $SrTiO_2$ and BaF_2 Induced by Impact of Slow Highly Charged Ions — •René Heller, Ayman S. El-Said, Richard A. Wilhelm, and Stefan Facsko — Helmholtz-Zentrum Dresden Rossendorf, Bautzner Landstr. 400, 01328 Dresden, Germany

The interaction of slow highly charged ions with solid surfaces with particular interest on the nano structure formation ability was investigated intensively within the last years. The rapid release of the HCI's potential energy as a unique feature of this kind of projectiles can cause local energy densities at the surface which are comparable to those induced by ultra short laser pulses or swift heavy ions.

Thus HCI give strong rise to be a promising tool for nano structure formation on solid surfaces. Since the potential energy release is strongly restricted to the surface proximity the amount of damage created in the bulk can be strongly suppressed.

In recent time the authors spend much effort in the exploration of the microscopic mechanisms of HCI nano structure creation on the surfaces of the alkali halide KBr and the earth alkali halide CaF_2, respectively. Motivated by the promising results and the predictions of the developed models we extended our investigation to the surfaces of $SrTiO_2$ as well as of BaF_2.

The results of these measurements are presented and discussed in the present contribution.

DS 42.11 Wed 15:00 P1

Electron exchange in a heterocycle-bridged biferrocene mixed-valence compound — •Nicolas Yèche[1], Yulia Krupskaya[2], Alexander Hildebrandt[3], Hans-Henning Klauss[1], Vladislav Kataev[2], and Heinrich Lang[3] — [1]Institut für Festkörperphysik ,TU Dresden — [2]Leibniz-Institut für Festkörper- und Werkstoffforschung Dresden — [3]Institut für Chemie, TU Chemnitz

Symmetrical systems comprising two or more metallocene units sometimes present interesting reduction and oxidation behavior: each of the metallocene unit can be separately oxidized/reduced, giving rise to intermediate valence compounds called "mixed valence" compounds. We present electrochemistry, magnetization, ESR and ^{57}Fe mössbauer spectroscopy measurement of a phenylpyridine bridged biferrocene compound in the mixed valence Fe(II)-Fe(III) state comparing it to normal Fe(II)-Fe(II) state. Resonance forms are observed in mössbauer spectroscopy at room temperature which indicates that the rate of the change between the Fe(II)-Fe(III) state and the Fe(III)-Fe(II) state is greater than 10^{-7}s. Further results and comarative analysis will be discussed.

DS 42.12 Wed 15:00 P1

Energy dependent spin scattering at a hybrid metal-organic interface — •Torsten Methfessel[1], Sabine Steil[2], Nicolas Grossmann[2], Kathrin Koffler[2], Martin Aeschlimann[2], Mirko Cinchetti[2], and Hans-Joachim Elmers[1] — [1]University of Mainz, Institute of Physics, D-55128 Mainz,Germany — [2]Department of Physics and Research Center OPTIMAS, University of Kaiserslautern, 67663 Kaiserslautern, Germany

In order to exploit the great potential of hybrid organic-inorganic interfaces for spintronics applications [1], fundamental knowledge about their spin-dependent properties is essential [2, 3]. We investigated the iron-copper phthalocyanine (CuPc) interface by means of spin polarized scanning tunneling spectroscopy (SP-STS) and spin polarized ultraviolet photoemission spectroscopy (SP-UPS). The combination of both techniques allows to measure the interface spin-dependent electronic properties in the energy region of relevance for spintronics applications. By comparing SP-STS and SP-UPS measurements on the Fe-CuPc interface we can distinguish two regions in the interface electronic structure: (i) In the first one (close to E_F) where no spin polarized hybrid interface states (SP-HISs) are present, the interface acts as a scattering barrier, characterized by an energy-independent spin-flip probability. (ii) In the second region, the spin-dependent tunnelling probability is dominated by SP-HISs, whose presence is confirmed by the SP-UPS measurements. [1] C. Barraud et al. Nat Phys 6 (2010) 615; [2] M. Cinchetti et al. PRL 104 (2010) 217602; [3] M. Cinchetti, et al. Nat Mater 8 (2009) 115.

DS 42.13 Wed 15:00 P1

Installation of a new variable temperature STM and measurements on Cobalt-Phthalocyanine — •Martha Scheffler, Torben Hänke, Danny Baumann, Ronny Schlegel, Dirk Bombor, Christian Hess, and Bernd Büchner — IFW Dresden, Institute for Solid State Research

A new scanning tunneling microscope was implemented in an existing chamber system and tested. It can be completely cooled by a liquid helium flow cryostat and can measure at temperatures down to 10K over a long period. Atomically resolved images as well as scanning tunneling spectroscopy with a high energy resolution can be obtained. Surface studies of Cobalt-Phthalocyanine molecules deposited onto HOPG and Au(001) surfaces will presented.

DS 42.14 Wed 15:00 P1

Organic-metal oxide hybrid thin film phototransistors — •Stephan Rossbauer[1], Stuart Thomas[2], Pichaya Pattanasattayavong[2], Peter Müller-Buschbaum[1], and Thomas D. Anthopoulos[2] — [1]TU München, Physik Department, LS Funkt. Mat., James-Franck-Str. 1, 85748 Garching, Germany — [2]Department of Physics and Centre for Plastic Electronics, Blackett Laboratory, Imperial College London, London SW7 2BW, United Kingdom

Metal oxide semiconductors are an interesting family of materials with great potential for a number of technological applications including transparent electronics, photovoltaics, smart windows and optical displays. This work presents the electronic and morphological effects of light-absorbing organic dyes functionalised directly onto the surface of zinc oxide (ZnO) based transistor channels produced by spray pyrolysis. Dynamic photo response is measured and discussed. The photosensitivity is tunable through the application of the gate voltage. The device produced can be used either as sensing device or as optoelectronic switch.

DS 42.15 Wed 15:00 P1

Dependence of Field-Effect Mobility on Semiconductor Layer Thickness in Organic Thin Film Transistors — •Christopher Keil and Schlettwein Derck — Institute of Applied Physics, Justus-Liebig-University Giessen, Germany. email:schlettwein@uni-giessen.de

Thin films of $F_{16}PcCu$ from the monolayer regime to thicker nm range were prepared under high vacuum conditions. As substrate a SiO_2 insulating layer was chosen. Metal contacts were evaporated as bottom contacts before the organic layer deposition. Organic thin film transistors of the molecular semiconductors were thereby achieved. Electrical conductivity as well as field-effect mobility were studied to investigate the role of the interface between the semiconductor and the gate insulator in bottom-gate field-effect transistors. The influence of organic film thickness as well as contact resistance between metal electrode and semiconductor layer were discussed to calculate the respective field effect mobility.

DS 42.16 Wed 15:00 P1

Thermally stimulated current measurements on P3HT based MIS-Diodes — •Tobias Könyves-Toth, Christian Melzer, and Heinz von Seggern — Electronic Materials Department, Institute of Materials Science Technische Universität Darmstadt, Petersenstraße 23, 64287 Darmstadt, Germany

Organic electronics show promising abilities even though there are still problems concerning lifetime and performance. These problems are often attributed to trap states in the volume of the employed organic semiconductor and to interface-near trap states. We report on interface traps occurring in state of the art poly(3-hexylthiophene) organic field-effect transistors (OFETs) examined by the technique of thermally stimulated currents (TSC). By using metal-insulator-semiconductor devices the sign of the applied voltage selects the accumulated charge carrier type at the interface and thus, hole or electron interface traps can be addressed. The contribution of the dielectric insulator on the TSC signal was unveiled by reference measurements on devices without the semiconducting layer. Utilizing the TSC method we were thus able to identify different trap states at the insulator-semiconductor and the semiconductor-contact interface and we will present the energetic distribution of the occupied density of states as measured by fractional TSC. Further, we will discuss whether trap states are induced by oxygen, as often stated in literature. The discussed results are crucial for the performance of OFETs as they affect the accumulated charge carriers in the transistor channel.

DS 42.17 Wed 15:00 P1

Organic field effect transistors on thin polyurethane films as gate dielectric — •Steffen Heuser, Jan Hartel, Christopher Keil, and Derck Schlettwein — Institute of Applied Physics, Justus-Liebig-University Giessen, Germany. email:schlettwein@uni-giessen.de

Thin insulating polymer layers (1 – 2.5 μm) of a two-component polyurethane resin were deposited by spin-coating as gate dielectric on a Pt gate electrode on poly(ethyleneterephthalate) PET. An interdigitated source and drain electrode array of gold was prepared to complete the setting of the measurement. Such structures with polymeric gate dielectrics are of interest to realize all-organic field effect transistors (OFET). In this study, 20 nm thin films of a perfluorinated phthalocyanine $F_{16}PcCu$ were prepared by physical vapour deposition (PVD) under fine vacuum conditions as an organic n-type semiconductor. The dielectric properties of the polymer insulating layer were determined by impedance spectroscopy. The transistor structures were measured and as characteristic properties the charge carrier mobility in the $F_{16}PcCu$ film, the threshold voltage and the on/off current ratio of the structures will be discussed.

DS 42.18 Wed 15:00 P1

Electrical and morphological characterization of self assembled nanofibers by means of conducting tip AFM — •Jörn-Oliver Vogel and Paolo Samorì — Institut de Science et d'Ingénierie Supramoléculaires, Strasbourg , Frankreich

Electrical and morphological characterization of self assembled nanofibers by means of conducting tip AFM

The simultaneous characterization of the morphology and the electronic properties of isolated nanostructures is important to understand how the spatial restrictions and the nanoscale order affect the electrical properties of nanoscale objects and organic electronic devices.

Here we report the study of the electrical properties of self organized nanofibers of poly(3-hexylthiophene) polymers adsorbed on an insulating substrate from a mixed p-xylene / chloroform solution.

The fibers were produced by means of spin-coating on a silicon oxide surface with pre-patterned gold electrodes. The P3ht fibers have a typical extension of 20 to 50 nm width, several um length, and 1.5 nm to 5 nm height. The IV characteristics of individual fibers are probed by the conductive AFM tip along the fiber contour in order explore the decay of current through this anisotropic nanostructure.

DS 42.19 Wed 15:00 P1

Integration of self-assembled photonic structures in excitonic solar cells — •Stefan Guldin[1], Sven Hüttner[1], Peter Kohn[1], Morgan Stefik[3], Pablo Docampo[2], Henry Snaith[2], Ulrich Wiesner[3], and Ullrich Steiner[1] — [1]Physics Department, Cavendish Laboratory, University of Cambridge, UK — [2]Physics Department, Clarendon Laboratory, University of Oxford, UK — [3]Materials Science Department, Cornell University, Ithaca, NY, USA

One way to successfully enhance light harvesting of excitonic solar cells in otherwise poorly absorbing spectral regions is the integration of optical elements in the device architecture. Recently concepts for the incorporation of one- or three-dimensional photonic crystal structures have been proposed which are geared towards enhancing absorption in specific parts of the optical spectrum while retaining the cell transparency.

In this work we present a novel route for the fabrication of a photonically active, mesoporous TiO_2 architecture from solution. The method relies on on the self assembly properties of the block copolymer PI-*b*-PEO in combination with sol-gel chemistry. When deposited in a layer-by-layer fashion, porosity and pore size of each individual coating can be controlled in detail, which enables the stacking of alternating high and low refractive index layers of TiO_2. The effects of such a highly reflecting one-dimensional photonic crystal on light absorption properties and cell efficiency of dye-sensitised solar cells will be discussed in detail.

DS 42.20 Wed 15:00 P1

Vertical Organic n-Triodes based on Me-PTCDI and fullerenes — •Axel Fischer, René Michel, Philipp Sebastian, Hans Kleemann, Alexander Zakhidov, Björn Lüssem, and Karl Leo — Institut für Angewandte Photophysik, George-Bähr-Straße 1, 01067 Dresden, Germany

Vertical Organic Triodes (VOT) are promising three terminal transistor devices, which, in contrast to organic field effect transistors (OFETs), can be processed in a vertical structure.

The major advantage of the vertical structure is the possibility to stack them with a second electronic device. For example, VOTs can be combined with an organic memory device to form an active matrix crossbar with the VOT as selection transistor. Due to stacking of the two devices, a high integration density can be achieved.

Furthermore, VOTs exhibit short active lengths which can be precisely controlled by the active layer thickness. Thus, these devices can drive high currents and high switching frequencies are in reach. Although considerable effort has been spent into the research of these devices, a detailed understanding of the working principles of these devices is still missing.

In this contribution, we will introduce the device concept of the VOT and discuss different electronic configurations. We will show organic triodes which are able to drive high current densities. Based on our results, we suggest that the working principle of the device is based on a permeable metal grid.

DS 42.21 Wed 15:00 P1

Charge transport simulations in amorphous organic materials — •Falk May and Denis Andrienko — Max-Planck-Institute for Polymer Research, Mainz, Germany

In the last few years organic materials have become a promising alternative to their inorganic counterparts in various applications for example in field effect transistors, photovoltaics and light emitting diodes. The advantage of using organic materials is due to a shear abundance of compounds that can be specially designed to meet different purposes, e.g. flexibility, light weight, or processability. However, many applications demand a high mobility of charge carriers and organic materials are still lacking behind their inorganic counterparts. Understanding the dynamics of charge carriers in organic materials is therefore a key question in the field, that we are currently addressing with the help of computer simulations in order to design new materials with improved mobilities[1]. We use a multi-scale approach starting from the description of (semi)-classical atomic interactions to generate a realistic morphology by molecular dynamics. At a higher length-scale we then describe charge carrier hopping through Marcus rates by including molecular interactions based on a quantum chemical calculation. On the largest length-scale we use kinetic Monte Carlo simulations to finally obtain charge carrier mobilities.

[1] X. Feng, V. Marcon, W. Pisula, M. R. Hansen, J. Kirkpatrick, F. Grozema, D. Andrienko, K. Kremer, K. Mullen, Nature Materials, 421-426, 2009

DS 42.22 Wed 15:00 P1

Donor-block-acceptor systems for photovoltaic applications — •Sven Hüttner[1], Michael Sommer[2], Kerr Johnson[1], Carol Huang[1], and Richard H. Friend[1] — [1]Cavendish Laboratory, University of Cambridge, UK — [2]Melville Laboratory, University of Cambridge, UK

Polymer solar cells rely on a donor and an acceptor material that form an interpenetrating morphology. This ensures charge separation at the interface, but also a proper charge percolation to the electrodes at the same time. Furthermore, the right position of HOMO and LUMO levels of the respective materials are important for an efficient charge separation. We present novel donor-block-acceptor polymers that can be applied in light harvesting devices. We want to control the heterojunction interface by these donor-block-acceptor molecules. These act as a phase compatibilizer to modify the polymer blend phase separation, but also affect the energetic environment of the heterojunction. Besides their structural characterisation, we investigated these materials by time-resolved spectroscopy. The donor-block-acceptor macromolecules contain P3HT as a donor block, and the acceptor block consists of perylene bisimide derivatives or F8TBT.

DS 42.23 Wed 15:00 P1

Characterization of bulk-heterojunction layers by imaging ellipsometry — •Christian Röling[1], Mathias Vaupel[2], Kristian O. Sylvester-Hvid[3], and Peter H. Thiesen[1] — [1]Accurion GmbH, Stresemannstr. 30, 37079 Göttingen — [2]Zeiss GmbH, Göttingen — [3]Riso National Laboratory for Sustainable Energy, DTU, Denmark

Conductive polymers and polymer-fullerene blends are promising materials for OLED and plastic solar cell applications. Blends prepared by two different methods, silk-printing and spin-coating were imaged, characterized and mapped using the spectroscopic imaging ellipsometer nanofilm_ep3se.

The optical characterization of bulk-heteroconjugate layers with imaging ellipsometry offers new information on the thickness distribution and refractive index distribution. Ellipsometric contrast micrographs are useful tools for the layer inspection concerning homogeneity and morphology, especially for the optimization of the coating process.

DS 42.24 Wed 15:00 P1

SXPS characterization of a donor / acceptor hetero junction for organic solar cells: High photovoltage at the merocyanine / fullerene interface — Eric Mankel, •Philip Reckers, Ludmila Konrad, Corinna Hein, Thomas Mayer, and Wolfram Jaegermann — Technische Universität Darmstadt, Materials Science Institute, Surface Science Division, Petersenstraße 32, 64287 Darmstadt, Germany

Novel absorber molecules are investigated for high efficient organic solar cells. Especially merocyanines provide high photovoltages as donor materials in photoactive organic hetero junction cells. The electronic alignment of a merocyanine / fullerene hetero junction is presented. The band diagram was determined by synchrotron induced photoelectron spectroscopy on in situ stepwise deposited fullerene on a merocyanine layer using the TGM7 dipole beamline at Bessy II. The merocyanine / fullerene HOMO offset is determined to be 850meV leading to a high LUMO offset, the driving force for exciton splitting. In situ bias illumination of the interface with 150W/m^2 of a halogen lamp leads to a reversible shift of the C60 emission features of about 800meV, indicating a high photovoltage. The height of the photovoltage depends on the fullerene layer thickness. It starts at 200mV for submonolayer coverage and increases up to approximately 1V for coverages of some ten nanometers.

DS 42.25 Wed 15:00 P1

Photodegradation of P3HT - a systematic study of environmental factors — •Holger Hintz[1], Ulf Dettinger[1], Hans-Joachim Egelhaaf[2], Larry Luer[3], Heiko Peisert[1], Thomas Chassé[1], and Jens Hauch[2] — [1]Eberhard-Karls-University, Institute for Physical and Theoretical Chemistry, Auf der Morgenstelle 8, D-72076 Tübingen, Germany — [2]Konarka Technologies GmbH, Landgrabenstr. 94, D-90443 Nürnberg, Germany — [3]Madrid Institute for Advanced Studies, IMDEA Nanociencia, Mòdulo 13; Avda Fco Tomas y Valiente, 7, 28049 Madrid, Spain

The influence of environmental factors on the degradation process of P3HT film has been investigated quantitatively. The decay kinetics of the polymer absorption during variation of intensity and spectral distribution of the incident light, oxygen concentration, humidity level as well as temperature are monitored using infrared and UV/VIS absorption spectroscopy. Oxygen diffusion into the polymer film has been investigated using fluorescence spectroscopy. The degradation process is light initiated with a strong increase of the effectiveness towards the ultraviolet region of the spectrum. The photo oxidation is not oxygen diffusion limited although an activation energy of 26 kJmol-1 was observed for both degradation and oxygen diffusion. The observed kinetics, especially its dependence on wavelength of the incident light, point to a radical- based degradation process in the solid state rather than a singlet oxygen based mechanism as it is observed in the liquid phase. The presence of humidity strongly affects the degradation process although water itself does not decompose the polymer.

DS 42.26 Wed 15:00 P1

Orientation and interface properties of a promising low bang gap polymer for organic solar cells — •Umut Aygül[1], David Batchelor[2], Ulf Dettinger[1], Heiko Peisert[1], and Thomas Chassé[1] — [1]Universität Tübingen, Institut für Physikalische und Theoretische Chemie, Auf der Morgenstelle 18, 72076 Tübingen — [2]Karlsruher Institut für Technologie, Institut für Synchrotron Strahlung, 76344 Eggenstein-Leopoldshafen

In polymer based bulk heterojunction-type solar cells so-called low band gap materials with alternating electron-deficient and electron-rich subunits are promising donor components in active layers to improve the efficiency of organic solar cells. A potential candidate in this context is Poly[2,6-(4,4-bis-(2-ethylhexyl)-4H-cyclopenta [2,1-b;3,4-b']dithiophene)-alt-4,7(2,1,3 benzothiadiazole) (PCPDTBT). The application of new materials requires a detailed understanding of the orientation and the electronic properties of the system and interface as these have a dramatic effect on device performance and efficiency. We study the electronic properties of interfaces between PCPDTBT and prototypical electrodes as well as between PCPDTBT and PCBM (acceptor) using X-ray photoemission spectroscopy (XPS) and valence band ultraviolet photoemission spectroscopy (UPS). Furthermore the preferred orientation of thin PCPDTBT films on both ITO and Si was studied with X-ray absorption spectroscopy (XAS) by looking at the sulphur K edge.

DS 42.27 Wed 15:00 P1

Charge Transport in Amorphous Oligothiophenes — •Manuel Schrader[1], Björn Baumeier[1], Chris Elschner[2], Moritz Riede[2], Karl Leo[2], and Denis Andrienko[1] — [1]Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany — [2]TU Dresden, Institute of Applied Photophysics, Mommsenstr. 13, 01062 Dresden, Germany

Organic semiconducting materials are needed for emerging devices such as photovoltaic solar cells. In this work we combine first principle calculations, molecular dynamics and kinetic Monte Carlo simulations to study charge transport in dicyanovinyl oligothiophenes of different lengths. Poole-Frenkel behavior of the charge carrier mobility is rationalized based on electrostatic and conformational disorder.

DS 42.28 Wed 15:00 P1

Hybrid Solar Cells made of Phthalocyanines and Zinc Oxide Nanowires — •Michael Kozlik, Steffen Milz, Sven Möller, Carsten Ronning, and Torsten Fritz — Institute of Solid State Physics, University of Jena, 07743 Jena, Germany

Hybrid Solar Cells are a topic of recent interest [1]. Usually the inorganic material is combined with organic polymers with increased interface area by using nanostructures. Our aim is to use the better photo current performance of small molecules, i.e. phthalocyanines [2], compared to polymers. Phthalocyanines show a high absorbance in the visible range, which is characterized by UV-Vis spectroscopy. The electronic ground state and the energetic level alignment were investigated using UV photoelectron spectroscopy. ZnO nanowires, synthesized by the vapor-liquid-solid route, are used due to the good conductivity and the transparency in the visible range [3]. A nearly perpendicular nanowire growth was achieved using a ZnO seed layer. The surface-to-volume ratio can be varied by changing the growth parameters. The morphology of the samples was investigated with scanning electron microscopy, while the atomic composition was obtained from X-ray analysis. The substrate and front contact were optimized to remain the high conductivity during nanowire growth. We will also present first results of a hybrid solar cell made of the combination of zinc oxide nanowires and phthalocyanines. References [1] S. Günes et al., Inorg. Chim. Acta 361 (2008) 581. [2] N. Papageorgiou et al., Prog. Surf. Sci. 77 (2004) 139. [3] C. Borchers et al., J. Phys. Chem. B. 110 (2006) 1656.

DS 42.29 Wed 15:00 P1

Influence of different solvents on the morphology in P3HT:PCBM bulk heterojunction systems for organic photovoltaics — •Shuai Guo[1], Matthias A. Ruderer[1], Volker Körstgens[1], Robert Meier[1], Hsin-Yin Chiang[1], Jan Perlich[2], and Peter Müller-Buschbaum[1] — [1]TU München, Physik Department, LS Funkt. Mat., James-Franck-Str. 1, 85748 Garching, Germany — [2]HASYLAB at DESY, 22603 Hamburg, Germany

Polymer-based photovoltaics have become of major interest in basic research as well as in application. One very promising system consists of poly(3-hexylthiophene) (P3HT) and the fullerene derivate PCBM. We investigate the morphology of bulk heterojunction films based on P3HT:PCBM. Films are cast from different solvents. It is well known that the solvent properties strongly influence the film formation and therefore influence the performance. In this work the surface structure is investigated by optical microscopy and AFM. In combination with scattering techniques such as XRR, GI(U)SAXS and GIWAXS, revealing the inner structure as well as the crystallinity, the whole morphology of the active layer is detected. Consequently, the different morphologies formed from different solvents are determined and compared with the corresponding performance of these systems.

DS 42.30 Wed 15:00 P1

Characterisation of Organic Field-Effect Transistors using Zinc Tetraphenylporphyrin Monomers and Dimers as Active Layers — •Iulia Genoveva Korodi[1], Daniel Lehmann[1], Simona Pop[2], Aoife Ryan[3], Mathias Senge[3], and Dietrich R. T. Zahn[1] — [1]Chemnitz University of Technology, Semiconductor Physics, D-09107 Chemnitz, Germany — [2]ISAS-Institute for Analytical Sciences, Albert-Einstein-Str.9, D-12489 Berlin, Germany — [3]School of Chemistry, SFI Tetrapyrrole Laboratory, Trinity College Dublin, Dublin 2, Irland

In this work bottom contact organic field-effect transistors (OFETs) using Zinc Tetraphenylporphyrin (ZnTPP) monomers and dimers as active layers were prepared and characterised. The ZnTPP dimer molecules are intramolecularly connected via a $C\equiv C$ bridge. The films were prepared by drop coating from a tetrahydrofuran solution on Si substrates with 100 nm SiO_2 on top with pre-structured gold contacts (from Fraunhofer IPMS Dresden). The channel lengths and the channel width defined by the lithography mask are $L = 2.5$ μm, 5 μm, 10 μm and 20 μm and $W = 10$ mm, respectively. The influence of using ZnTPP monomers or dimers on the on/off ratio, threshold voltage and charge carrier mobility is compared and discussed. The effect of the morphology as revealed by the scanning electron microscopy images is discussed as well.

DS 42.31 Wed 15:00 P1

Time resolved microwave conductivity measurements of Bulk Heterojunction solar cells — •Shine Philip[1], Elias Martinez[2], Klaus Müller[1], Marinus Kunst[2], and Dieter Schmeisser[1] — [1]Brandenburg University of Technology, Department of Applied Physics and sensors, K.-Wachsmann-Allee 17, 03046, Cottbus, Germany — [2]Helmholtz- Zentrum Berlin for Materials and Energy, Hahn-Meitner-Platz 1, 14109 Berlin Germany

The time resolved microwave conductivity (TRMC) method was used in order to study the generation and decay kinetics of charge carriers in the Bulk Heterojunction (BHJ) solar cells. The charge carriers were generated with 532nm laser pulses of 10ns FWHM (Full Width at Half Maximum) induced in the cells. The BHJ solar cells used for the measurements had a photoactive layer consisting of a mixture of Poly (3-Hexylthiophene) P3HT and Phenyl-C61-butyric acid methyl ester (PCBM) which was spin coated onto Indium tin oxide (ITO)/glass substrates. In the field of Organic photovoltaic blends, TRMC method is introduced as a new method of direct investigation of the charge carrier lifetime as well as the charge carrier mobility and we were successful in studying the charge carrier lifetime of the reference BHJ solar cells. We also studied the influence of aligned ferroelectric fields on the charge separation in BHJ solar cells. As ferroelectric material, we used the copolymer Poly (vinylidene fluoride - trifluoroethylene) P(VDF-TrFE).

DS 42.32 Wed 15:00 P1

Sol-Gel Templated Zinc oxide Films for Solar Cell Application — •Kuhu Sarkar and Peter Müller-Buschbaum — TU München, Physik Department, LS Funkt. Mat., James-Franck-Str. 1, 85748 Garching, Germany

Hybrid solar cells consisting of both the organic and the inorganic semiconductor parts are a potential source for low cost green electricity. The organic conjugated polymer acts as a hole-conducting material while the inorganic oxide as an electron acceptor. The nanostructured morphology of inorganic material in the hybrid solar cells leads to enhanced device performance by increasing the active surface area for interfacial interactions. Among the various inorganic metal oxides, zinc oxide is a promising material for use in hybrid solar cells on account of its high electron mobility, a direct band gap of 3.37 eV at room temperature, large excitons binding energy, excellent chemical and thermal stability, suitable optical properties and environment-friendly behaviour. A sol gel approach based on an amphiphilic diblock copolymer acting as a structure directing agent is used to obtain a ZnO network structure via spin coating. Primary structural investigation of the films is carried out using SEM and AFM.

DS 42.33 Wed 15:00 P1

Evaluation of Barrier Films for Organic Solar Cells Using an Electrical Calcium-Test — •Hannes Klumbies[1], Sylvio Schubert[1], Lars Müller-Meskamp[1], Olaf R. Hild[2], and Karl Leo[1,2] — [1]Institut für Angewandte Photophysik, Dresdner Innovationszentrum Energieeffizienz, TU Dresden, 01062 Dresden, Germany

— [2]Fraunhofer Institute for Photonic Microsystems, 01109 Dresden, Germany

In contrast to common solar cells based on silicon, organic solar cells have the potential to be cheap and flexible. The latter is especially important for mass-production (Roll-to-Roll-processing), mobile applications and low-cost, lightweight installations. However, flexibility poses a challenge for stable encapsulation of the organic solar cell to prevent it from degradation due to oxygen and water vapor. It is common agreement that the transmission rates for these species should be 1E-4 g/m^2*d or lower - four to five orders of magnitude below the rate of a typical polymer foil. Transmission rates that low are not only difficult to achieve but also difficult to measure. Ready-to-use commercial devices based on coulometry only reach a sensitivity of 5E-4 g/m^2*d.

In this work we use an electrical Ca-test as a sensor for water vapor and oxygen. Its sensitivity is in the range of 5E-5 g/m^2*d or better.

Furthermore we show water-vapour-transmission-rates achieved by different barrier layers on polymer-foil, e. g. sputtered oxides, and compare them with the rates achieved by bare polymer- and commercial barrier-foils.

DS 42.34 Wed 15:00 P1

Solution-processable organic light emitting diode on glass fibers for textile applications — •Björn Gruber, Schulze Kerstin, and Janietz Silvia — Fraunhofer Institute for Applied Polymer Research, Geiselbergstr. 69, 14476 Potsdam-Golm, Germany

Electronic devices based on organic materials offers the possibility to be a low-cost production technology on large area in several years. As a special application organic devices could be used in the field of electronic-textiles in future, for example for safety applications or as smart textiles. Therefore the direct integration of the electronic devices on the textile fibers is interesting.

In this work, organic light emitting diodes (OLEDs) have been manufactured and investigated on cylindrical and flexible substrates. Especially the cylindrical geometry of the substrate hinders a homogeneous deposition of organic layers. Here, we present first results using solution processes for the preparation of the organic materials of an organic light emitting diode on glass fibers. The OLEDs were prepared on thin glass fibers using thermally evaporated metals and dip-coated polymeric layers. We focus on the challenging preparation steps of these layers on cylindrical substrates resulting in working devices. Additionally a current density-voltage-characteristic of a light emitting device on a glass fiber is presented and analyzed.

DS 42.35 Wed 15:00 P1

Inkjet printing of organic layers on nano- and microstructured flexible substrates for organic electronic devices — •Marcel Schmidt[1], Peter Lewer[1], Kerstin Schulze[1], Silvia Janietz[1], Felix Stelzl[2], Chegnui Bekeny[2], and Uli Würfel[2] — [1]Fraunhofer Institute for Applied Polymer Research, Geiselbergstr. 69, 14476 Potsdam-Golm, Germany — [2]Fraunhofer Institute for Solar Energy Systems, Heidenhofstr. 2, 79110 Freiburg, Germany

Inkjet printing as deposition method for organic materials in electronic devices promises to be a low-cost production technology in future. The advantage of this technique is the ability to deposit a small amount of material on defined areas on substrates, e.g. for the preparation of organic field effect transistors (OFETs) or organic solar cells (OSCs). As a special application the use of 3D-nanostructured electrodes on flexible substrates as a high voltage source could be already demonstrated [Adv. Mater. 20, 4055]. The deposition of material layers is especially influenced by the capillary forces of the electrode structures and by the formation of inhomogeneous layers. Here, we present our results on the development of an inkjet printing process for semiconductor materials on nano- and microstructured substrates. The capillary forces resulting from the structure of the substrates as well as the solvents of the ink were examined for the development of the printing process. The prepared layers were analysed using atomic force microscopy (AFM) and scanning electron microscopy (SEM). The fabrication of smooth layers within the microstructure will be demonstrated as well as first results of photovoltaic cells on nanostructured substrates.

DS 42.36 Wed 15:00 P1

Photoelectron Spectroscopy Investigation of the C60/Calcium Interface — •Holger Wetzstein[1], Darius Bunandar[2], Julia Schafferhans[3], Carsten Deibel[3], Achim Schöll[1], and Friedrich Reinert[1] — [1]Experimental Physics VII, Julius-Maximilians-University of Würzburg, D-97074 Würzburg — [2]Department of Physics, University of Texas at Austin, Austin, Tx 78712-0264 — [3]Experimental Physics VI, Julius-Maximilians-University of Würzburg, D-97074 Würzburg

Device lifetime is a crucial point for organic solar cells. Therefore it is important to understand the degradation mechanisms as well as their consequence on the performance of these photovoltaic devices. We observed a characteristic S-shape in the I/V-curves of P3HT/PCBM-bulk heterojunction cells with calcium contacts. A tentative origin of this behavior is a reaction of the calcium with oxygen, which leads to alterations in the regime of the anode interface. To shed more light on this issue we investigated the electronic structure of the Ca/C60 interface, which serves as a model for the PCBM/Ca contact. X-ray (XPS) and ultra-violet photoelectron spectroscopy (UPS) measurements were performed on C60 layers adsorbed on epitaxially grown Calcium as well as on Ca deposited on C60. In both cases, the data clearly show the formation of an interface state due to the charge transfer from the Ca into the C60, which is an indication for a chemical reaction. Moreover, we studied the effect of oxygen exposure on the interfacial chemical and electronic structure under conditions comparable to the conditions during device operation.

DS 42.37 Wed 15:00 P1

Determination of molecular electronic excitations using epitaxial thin film growth: Perfluoropentacene on alkali halides — •Tobias Breuer and Gregor Witte — Molekulare Festkörperphysik, Philipps-Universität Marburg, D-35032 Marburg

The study of optical excitations is an important part of understanding electronic properties in organic semiconductors. As it is in many cases hardly possible to prepare sufficiently sized crystals, optical spectroscopy of organic single crystals is a challenging topic. Here we present an alternative approach: to study optical excitations in Perfluoropentacene ($C_{22}F_{14}$) we prepared epitaxial thin films on the (100)-surfaces of alkali halides. The epitaxial growth of PFP films was proved and studied by AFM and XRD measurements. While exhibiting the same crystalline phase a rather different molecular orientation is adopted on both substrates showing an upright orientation on NaF and a recumbent orientation on KCl which in both cases are stabilized by an electrostatic point-in-line relationship between the outermost fluorine atoms and the alkali cations of the substrate surfaces. While previous studies of optical excitations in PFP were hampered by the laterally isotropic (100)-growth of PFP on amorphous SiO_2[1] the different epitaxial growth modes on the alkali halides enabled access to all molecular axes. A combination of UV/Vis measurements and spectrally and polarization resolved microscopy enabled the determination of the polarization dependence of the observed optical excitations. Evidence of intermolecular coupling was found and will be discussed.

[1] A. Hinderhofer et al., J. Chem. Phys. 127, 194705 (2007).

DS 42.38 Wed 15:00 P1

IR-Spectroscopy on organic charge-transfer complexes — Sebastian Beck[1], •Milan Alt[1], Tobias Glaser[1], Akemi Tamanai[1], Diana Nanova[1], Michael Kröger[2], and Annemarie Pucci[1] — [1]Kirchhoff-Institut für Physik, Universität Heidelberg — [2]InnovationLab GmbH, Heidelberg

In the ongoing development of organic electronic devices new materials with adjustable properties are needed, in order to meet different specific requirements. Prototypical examples are the CT-complexes, such as TTF-TCNQ and its derivates. We studied the optical properties of these CT-complexes in the whole infrared range (100 - 12000 cm^{-1}). The suggested linear relationship between the excitation energy of the C-N-stretching vibration of the acceptor TCNQ and the associated charge-transfer was verified. In addition to the vibronic excitations of the molecules also widely broadened absorption bands in the MIR and NIR were observed. These are attributed to electronic excitations and in the range of the HOMO-LUMO gap of the investigated complexes.

DS 42.39 Wed 15:00 P1

IR studies on an emitter/host mixture — •Tobias Glaser[1], Christian Lennartz[2], Christian Schildknecht[2], and Annemarie Pucci[1] — [1]Kirchhoff-Institut für Physik, Universität Heidelberg — [2]BASF SE, Ludwigshafen

In this study, we show how infrared spectroscopy can be used to investigate the mixing of two organic materials. The materials, in this case a phosphorescent emitter that was developed for organic light emitting devices and a suitable host material, were deposited by vapour sublimation under ultra-high vacuum conditions. By comparing the experimental spectra of thin layers of the pure materials to quantum chemical calculations, the calculated vibrational modes could be assigned to the measured absorption bands. Embedding the emitter into the host by simultaneous evaporation of these two materials gives rise to only small changes in the relative intensity of the IR absorption bands due to the change in background polarisability, but significantly effects the photoluminescence.

DS 42.40 Wed 15:00 P1

Structure and morphology of co-evaporated pentacene-perfluoropentacene thin films[1] — •Christian Frank[1], Alexander Hinderhofer[1], Takuya Hosokai[1], Andrea Resta[2], Alexander Gerlach[1], and Frank Schreiber[1] — [1]Institut für Angewandte Physik, Universität Tübingen, Auf der Morgenstelle 10, 72076 Tübingen, Germany — [2]ESRF, BP 220, F-38043 Grenoble, France

The morphology as well as the structure of thin films, consisting of pentacene (PEN) and perfluoropentacene (PFP)[2] binary blends on SiO_2, were investigated by means of x-ray reflectivity and grazing incidence x-ray diffraction. Furthermore, reciprocal space maps of these blends with different volume fractions show the co-existence of two intermixing phases in addition to pure PEN and PFP crystallites. The question whether these intermixing occurs on a molecular length scale is addressed. The σ-phase, with its long molecular axis nearly perpendicular to the substrate, is thermally stable and nucleates predominantly at high temperatures. The λ-phase (long molecular axis nearly parallel to the substrate) exhibits a growth behavior, which is enhanced by low temperatures. Additionally, both phases can tentatively be identified within the reciprocal space maps.
[1] A. Hinderhofer, C. Frank, T. Hosokai, A. Resta, A. Gerlach, F. Schreiber, **submitted**
[2] A. Hinderhofer, U. Heinemeyer, A. Gerlach, S. Kowarik, R. M. J. Jacobs, Y. Sakamoto, T. Suzuki, F. Schreiber, J. Chem. Phys. **127**, 194705 (2007)

DS 42.41 Wed 15:00 P1

Structural and Vibrational Properties of C_{60} Fullerene Thin Films on Gold Surfaces — •Caroline Henneke, Philip Schulz, Tobias Schäfer, and Matthias Wuttig — I. Physikalisches Institut (IA), RWTH Aachen University, Germany

The fullerene C_{60} is a widely employed acceptor material for organic solar cells. By tailoring the structure of C_{60} thin films and thus tuning their properties the efficiency of C_{60}-based solar cells can be improved. However, it remains a main challenge to determine the correlation between the structure of C_{60} thin films and their optoelectronic properties.
Here, the influence of substrate temperature during deposition in a vacuum thermal evaporation process (VTE) on the structure and vibrational properties of C_{60} thin films on Au surfaces is investigated. Substrate temperatures ranging from 150 K to 700 K were applied in this study. XRD measurements were conducted to identify structural changes in the C_{60} thin films, while the surface morphology was determined by AFM measurements. The vibrational characteristics of the C_{60} thin films were investigated by Fourier-Transform Infrared spectroscopy (FTIR).

DS 42.42 Wed 15:00 P1

Analysis of structure and electronic alignment of PTCDI-C13 thin films on metal surfaces — •Daniel Gebauer, Philip Schulz, Dominik Meyer, Christian Effertz, and Matthias Wuttig — RWTH Aachen, I. Institute of Physics (IA), D-52056 Aachen, Germany

N,N'-Ditridecylperylene-3,4,9,10-tetracarboxylic diimide (PTCDIC13) depicts a potential acceptor material for organic solar cells. To understand the mechanisms of film formation and charge carrier transfer, it is necessary to examine the interface effects between the organic layer and the metal contact.

In this study thin films of PTCDI-C13 with a thickness varying from single monolayers to 20 nm, are evaporated on Au, Ag, Cu, and Al substrates. The energy level alignment between the valence band of each metal and the molecular orbitals of the subsequently deposited organic layer is analyzed by Ultraviolet Photoelectron Spectroscopy (UPS). Structure and surface morphology of the PTCDI-C13 films have been investigated by Atomic Force Microscopy (AFM) and X-Ray Diffractometry (XRD) in order to study the growth behavior of these films.

DS 42.43 Wed 15:00 P1

Tetrazine Thin Film Growth on SAM-coated Gold Surfaces — •Dominik Meyer[1], Philip Schulz[1], Laurent Galmiche[2], Pierre Audebert[2], and Matthias Wuttig[1] — [1]Institute of Physics (IA), RWTH Aachen University of Technology, 52056 Aachen, Germany — [2]P.P.S.M. (CNRS UMS 8531), École Normale Supérieure de Cachan, 61 Avenue du Président Wilson, 94235 Cachan Cedex, France

The modification of noble metal surfaces by organosulfur self-assembled monolayers (SAM) is a widely studied topic in the field of organic optoelectronics. The assembly of such monolayers alters the electronic structure of the metal surface and strongly affects thin film growth of subsequently deposited organic material employed in optoelectronic devices. Here we present the impact of SAMs on the crystal growth of 3,6-bis(3,5-dimethylpyrazol-1-yl)-1,2,4,5-tetrazine (bpytz). Tetrazines are promising candidates as alternative active materials for optoelectronic and sensor applications as they generally provide a high electron affinity. This study compares the growth of bpytz on pure Au(111) surfaces with modified gold surfaces employing decanethiol and didecyl-dithiocarbamates as self-assembling monolayers. X-ray diffraction (XRD) and Infrared (IR) spectroscopy are employed to investigate the different growth scenarios, while density functional theory (DFT) was utilized to analyze the measured IR data.

DS 42.44 Wed 15:00 P1

Infrared Spectroscopic Ellipsometry Measurements of Polytriarylamine (PTAA) Thin Films — Jens Trollmann, Robert Lovrincic, •Akemi Tamanai, and Annemarie Pucci — Im Neuenheimer Feld 227, 69120 Heidelberg, Germany

Organic materials have been adopted for thin film fabrications since organic molecules are less expensive to produce, and high light absorbing capacity can be expected. For improving the electrical performance, investigation of the dielectric properties for the organic thin films is essential, hence Ψ and Δ measurements have been performed by means of spectroscopic ellipsometry (SE) (Woollam IR-VASE) so as to determine highly accurate dielectric constants (real and imaginary part) and thickness of polytriarylamine (PTAA) thin films (produced by Merck) in the infrared (IR) spectral range between 350 and 5500 cm^{-1}. PTAA is an extraordinarily stable p-type semiconductor material which can be handled in air, high field-effect mobility of organic field-effect transistors (OFETs) fabricated together with PTAA and a low k insulator (low k dielectrics) has been reported. It is possible to obtain the bands not only from molecular vibrations, but also from excitations of free carriers with the SE which dominate the dielectric response of semiconductor thin films in the IR region.

DS 42.45 Wed 15:00 P1

Charge carrier mobility in different donor materials for polymer solar cells — •Oleisa Synooka, Chetan Raj Singh, Marco Seeland, Gerhard Gobsch, and Harald Hoppe — Institüt für Physik, TU Ilmenau, Weimarer str.32, 98693 Ilmenau, Germany

Abstract: During recent years, many donor materials of varying band gap have been synthesized for polymer solar cell applications. Here, we compare the charge carrier mobilities of different commercially available p-type materials (e.g. P3HT and- PCDTBT) by the Space Charge Limited Current (SCLC) method. The mobility measurement results from SCLC are compared with Charge Extraction by Linearly Increasing Voltage (CELIV) measurements. Furthermore, several anode materials (e.g. PEDOT:PSS) have been investigated and compared with respect to their charge injection behavior.

DS 42.46 Wed 15:00 P1

In-situ protein adsorption study using spectroscopic IR-ellipsometry — •Philipp Gehlich, Andreas Furchner, Karsten Hinrichs, Norbert Esser, and Dennis Aulich — Leibniz-Institut für Analytische Wissenschaften - ISAS - e.V.; Albert-Einstein-Str. 9; 12489 Berlin; Germany

In-situ IR-ellipsometry was used to determine the differences in absorption spectra of bovine serum albumin (BSA) films on silicon in aqueous solution. A special flow-cell [1,2] which allows to record spectra at varying temperatures was employed. At an incident angle of 50° tan Ψ - spectra were recorded at different times of the adsorption process. Amide-I- and, partially, amide-II-bands of the thin protein film could be identified and a variation was monitored until the adsorption process was completed. References: [1] K. Hinrichs, K. Roodenko and J. Rappich, Electrochem. Commun. 10 (2008), p. 315.; [2] Y. Mikhaylova, L. Ionov, J. Rappich, M. Gensch, N. Esser, S. Minko, K.-

J. Eichhorn, M. Stamm and K. Hinrichs, Anal. Chem. 79 (2007), p. 7676.

DS 42.47 Wed 15:00 P1

Structure and optical properties of binary co-evaporated organic thin films: Diindenoperylene and Perfluoropentacene — •Jens Reinhardt, Alexander Hinderhofer, Katharina Broch, Ute Heinemeyer, Alexander Gerlach, and Frank Schreiber — Institut für Angewandte Physik, Universität Tübingen, Auf der Morgenstelle 10, 72076 Tübingen, Germany

The structural and optical properties of co-evaporated thin films of diindenoperylene[1] (DIP) and perfluoropentacene[2] (PFP) on SiO_2 and glass-substrates were studied using x-ray reflectivity, grazing incidence x-ray diffraction, differential reflection spectroscopy (DRS), and absorption spectroscopy. The x-ray data reveal the coexistence of at least one molecular mixed DIP:PFP phase distinct from the pure DIP and PFP thin film phases. In addition the absorption and DRS spectra of the mixture cannot be described by a superposition of the single-component spectra which is attributed to different intermolecular coupling. A systematic variation of growth parameters (substrate temperature: 300 - 360 K; thickness: 5 - 40 nm) and their effect on phase mixing/separation will be discussed.

[1] U. Heinemeyer *et al.*, Phys. Rev. B, **78** (2008) 085210

[2] A. Hinderhofer *et al.*, J. Chem. Phys., **127** (2007) 194705

DS 42.48 Wed 15:00 P1

Molecular anchoring on metal surfaces — Albano Cossaro[2], Dean Cvetko[1,3], Luca Floreano[2], •Michele Puppin[1,2,4], Alberto Verdini[2], and Alberto Morgante[1,2] — [1]Department of Physics, University of Trieste, Trieste, Italy — [2]CNR-IOM, Laboratorio TASC, Trieste, Italy — [3]Department of Physics, University of Ljubljana, Ljubljana, Slovenia — [4]Department of Physical Chemistry, Fritz Haber Institut der Max Planck Gesellschaft, Berlin, Germany

The possibility to control the structural properties of interface layers of an organo-metallic system is a major task of nano-devices engineering. In many cases, a Self Assembled Monolayer (SAM) is used for anchoring molecules or proteins to the substrate or, in organic electronics, for modifying the surface of metallic electrodes in contact with the organic active layers. The Au(111) surface can be functionalized with amine (-NH2) groups by growing a SAM of cysteamine in ultra-high vacuum. The modified surface is used to anchor molecules with a carboxylic (-COOH) functional group. The amine binds to the carboxylic group leading to a second layer in which the anchored molecules have a well defined orientation. To describe the formation and the final geometry of the organic structure we used XPS (X-ray Photoelectron Spectroscopy) and NEXAFS (Near Edge X-ray Absorption Fine Structure) spectroscopies.

DS 42.49 Wed 15:00 P1

Thin films of ethyne-linked porphyrin dimers investigated by spectroscopic ellipsometry — •Simona Pop[1], Peter Kate[1], Aoife Ryan[2], Xin Zhang[3], Jörg Rappich[3], Norbert Esser[1], Karsten Hinrichs[1], and Mathias Senge[2] — [1]Leibniz - Institut für Analytische Wissenschaften - ISAS - e.V., Albert-Einstein-Str.9, D-12489 Berlin, Germany — [2]School of Chemistry, SFI Tetrapyrrole Laboratory, Trinity College Dublin, Dublin 2, Ireland — [3]Helmholtz-Zentrum Berlin for Materials and Energy GmbH, Institute for Silicon Photovoltaics, Kekuléstrasse 5, Berlin, 12489, Germany

Thin films of ethyne-bridged porphyrin dimers are investigated by means of spectroscopic ellipsometry in the NIR-Vis spectral range. The porphyrin films were prepared on silicon substrates covered by the native oxide. For a better understanding of the optical behaviour of the porphyrin dimers, their corresponding monomers are additionally characterized. The dielectric functions of the porphyrin monomers and dimers are derived from ellipsometrical measurements by employing a three-phase optical model. The optical response of the porphyrin dimers is mainly characterized by red-shifts of the first absorption structure, Q-band, as well as by strong changes in the Q/B ratios, compared to the corresponding porphyrin monomers.

DS 42.50 Wed 15:00 P1

Characterization of temperature-sensitive swelling behavior of PNIPAAm brushes via in-situ infrared ellipsometry — •Andreas Furchner[1], Dennis Aulich[1], Eva Bittrich[2], and Karsten Hinrichs[1] — [1]Leibniz-Institut für Analytische Wissenschaften - ISAS - e. V. — [2]Leibniz-Institut für Polymerforschung Dresden e. V.

Over the last years, polymer brushes have received growing attention owing to their stimuli-responsive surface properties. In particular, mixed brushes, consisting of at least two different polymers, are interesting, since they represent biofunctional surfaces for controlled protein and cell adsorption due to stimuli-responsive behavior on changes in, for example, temperature, pH, or solvent.

Infrared Spectroscopic Ellipsometry (IRSE), a method for studying film properties at the solid-liquid interface, allows to study the structural and chemical properties of polymer layers and therefore makes it possible to tune mixed brush systems to the specific needs.

As an intermediate step towards a better understanding of mixed temperature-sensitive brushes, poly(N-isopropyl acrylamide) (PNIPAAm) mono-brushes were investigated using ex-situ as well as in-situ SE. The information about optical and structural properties obtained by fitting SE data to an appropriate optical layer model were then used to characterize the temperature-sensitive swelling behavior of PNIPAAm brushes.

DS 42.51 Wed 15:00 P1

Vibrational Properties of Metal Phthalocyanine Thin Films — •Michael Ludemann[1], Iulia E. Brumboiu[1,2], Ovidiu D. Gordan[1], Vasile Chiş[2], and Dietrich R. T. Zahn[1] — [1]Semiconductor Physics, Chemnitz University of Technology — [2]Faculty of Physics, Babeş-Bolyai University, Cluj-Napoca

In this work experimental Raman spectra of several phthalocyanine (Pc) molecules with different central metal atoms (Cu, Co, Fe and Ni) are compared to DFT calculations. Besides symmetry aspects the calculated and measured relative shifts of the vibrational bands due to the different central metal atoms provide additional information utilized to assign the measured Raman modes.

All samples were prepared by organic molecular deposition (OMBD) in ultra-high vacuum conditions (UHV). The measurements are performed *in situ* during growth or stepwise at fixed film thicknesses. For a better comparison to single molecule calculations Raman spectra at ultra-low coverage were measured.

DS 42.52 Wed 15:00 P1

Broadband dielectric spectroscopic studies on 4- heptan - 4'- isothiocyanatobiphenyl (7BT) in confining geometry. — •Malgorzata Jasiurkowska[1], Emmanuel U. Mapesa[1], Ciprian Iacob[1], Periklis Papadopoulos[1], Friedrich Kremer[1], and Maria Massalska-Arodz[2] — [1]Institute of Experimental Physics I, University of Leipzig, 04103 Leipzig, Germany — [2]The Henryk Niewodniczanski Institute of Nuclear Physics Polish Academy of Sciences, Radzikowskiego 152, 31-342 Kraków, Poland

Band Dielectric Spectroscopy is employed to investigate 4-heptan-4'- isothiocyanatobiphenyl (abbreviated as 7BT) in one- and two-dimensional confinement (in the frequency range 0.1 Hz to 10-6 Hz). In bulk, only one liquid crystalline phase, the smectic E (SmE) phase with orthorhombic arrangement within the molecular layers is observed. The bulk dielectric properties of the nBT compounds are now well understood. For measurements under one-dimensional confinement, ultrathin films of 7BT prepared by spin-coating method are measured in the nanostructured-electrode configuration. In contrast to bulk dielectric spectra where only one process is observed in the low frequency regime, an additional process appears. Dynamic properties of 7BT are also studied in nanoporous silica membranes. It is observed that the crystallization temperature is significantly reduced in comparison to the value for bulk 7BT. Moreover, beside the relaxation around short axis, two extra processes are observed. The influence of pore size on molecular dynamics will be discussed.

DS 42.53 Wed 15:00 P1

Density-Dependent Reorientation and Rehybridization of the Strongly Chemisorbed Conjugated Molecule Hexaazatriphenylene-hexacarbonitrile (HATCN) on Ag(111) — •A. Vollmer[1], B. Bröker[2], O. T. Hofmann[3], G. M. Rangger[3], P. Frank[3], R.-P. Blum[2], R. Rieger[4], L. Venema[5], H. Glowatzki[2], K. Müllen[4], J. P. Rabe[2], A. Winkler[3], P. Rudolf[5], E. Zojer[3], and N. Koch[2,1] — [1]Helmholtz Zentrum Berlin für Materialien und Energie GmbH, Germany — [2]Institut für Physik, Humboldt-Universität zu Berlin, Germany — [3]Institute of Solid State Physics, Graz University of Technology, Austria — [4]MPI für Polymerforschung, Mainz, Germany — [5]Zernike Institute for Advanced Materials, Groningen, The Netherlands

Understanding the fundamental electronic and morphological properties of interfaces between metals and conjugated organic materials

(COM) is crucial in the field of organic electronics. Hitherto, it has been commonly accepted that the orientation of a COM monolayer on a metal surface depends only on the strength of metal-molecule vs. intermolecular interactions. Here we show that a re-orientation of a face-on to an edge-on first layer can be triggered by increasing the amount of deposited molecules. We will report on the strong molecular acceptor HATCN on Ag(111), where this rearrangement is facilitated through the molecular cyano groups and accompanied by a rehybridization of molecular and metal electronic states, significantly modifying the interface and surface electronic properties. We will present UPS, $\Delta\Phi$, TDS, RAIRS, STM, and DFT. PRL,104,23,(2010), Nano Lett,8,11,(2008)

DS 42.54 Wed 15:00 P1

Chemical transformation of chloroaluminum phthalocyanine films upon post deposition annealing in magnetic field — Tamara Basova[1], Vladimir Plyashkevich[1], •Fotini Petraki[2], Heiko Peisert[2], and Thomas Chassé[2] — [1]Laboratory for chemistry of volatile and metallorganic compounds, Nikolaev Institute of Inorganic Chemistry, Siberian Branch Russian Academy of Science, 630090, Lavrentiev ave.3, Novosibirsk, Russian Federation — [2]Universität Tübingen, IPTC, Auf der Morgenstelle 18, 72076 Tübingen, Germany

The annealing of chloroaluminum(III)phthalocyanine (AlClPc) thin films in air results in a chemical transformation to μ-(oxo)bis[phthalocyaninato] aluminum(III) ((AlPc)2O). A comparative analysis of the influence of post deposition annealing process without and under applied magnetic field of 1 T, on the composition and morphology of AlClPc films, has been carried out. The chemical transformation of AlClPc to (AlPc)2O on the substrate surface is studied using UV-vis and Infrared (IR) spectroscopies, Raman, X-ray photoelectron spectroscopy (XPS) as well as atomic force microscopy (AFM). Two interesting effects were observed upon heating the AlClPc films in magnetic field of 1 T: First, the temperature of the chemical transformation of AlClPc to (AlPc)2O decreases from 300 to 200 °C, when magnetic field was applied during post deposition annealing. Second, the formation of (AlPc)2O films with elongated crystallites with a preferential orientation was observed. The heating of (AlPc)2O films in the magnetic field at the same conditions did not demonstrate any effect on structure and morphology of these films.

DS 42.55 Wed 15:00 P1

Second-Harmonic Generation Spectroscopy of Magnesium Tetraphenylporphyrin Films — •Jan Metje[1,2], Gerhard Lilienkamp[1], and Winfried Daum[1,2] — [1]Institute for Energy Research and Physical Technologies, TU Clausthal, Leibnizstr. 4, 38678 Clausthal-Zellerfeld — [2]NTH School for Contacts in Nanosystems

Porphyrins such as magnesium tetraphenylporphyrin (MgTPP) are widely known as energy harvester in biological energy cycles. More recently, their efficient conversion of photonic energy has triggered their use as sensitizers in solar cells. The strong absorption of light by porphyrin molecules in the blue-to-violet spectral range is due to the molecular $S_0 \rightarrow S_2$ excitation which gives rise to so-called Soret bands in absorption experiments. While the spectral position and width of these bands are rather insensitive to a substitution of the central atom (Mg, Zn, 2H), the spectra strongly depend on the local environment of the molecule. In this contribution we report on second-harmonic generation (SHG) experiments performed with MgTPP films evaporated on SiO_2 under ultra-high vacuum conditions. SHG spectra of MgTPP films in the spectral range of the Soret band show two bands with energies at 2.94 eV (422 nm) and 2.7 eV (460 nm). The spectral position of the former band agrees with that of individual MgTPP molecules dissolved in solutions whereas the large red shift of the latter band indicates strong intermolecular interactions. Results of SHG experiments with MgTPP films of different thicknesses will be presented to verify the surface and bulk character, respectively, of these molecular excitations.

DS 42.56 Wed 15:00 P1

Epitaxial Growth of Lead-Phthalocyanine on GaAs(001) Reconstructed Surfaces — •Linda Riele[1], Benjamin Buick[1], Thomas Bruhn[2], Bjørn-Ove Fimland[3], Patrick Vogt[2], and Wolfgang Richter[1] — [1]Università di Roma Tor Vergata, Rome, Italy — [2]TU Berlin, Berlin, Germany — [3]Dept. of Electronics and Telecommunications, NTNU, Trondheim, Norway

Heterostructures of semiconductors and metal substituted phthalocyanine (MPc) films have attracted growing scientific and industrial interest because of their application in opto- or electronic devices. An important aspect in this respect is the control of the molecular ordering within the organic layers since the electrical conductivity of these layer depends crucially on the orientation and ordering of the molecules. Here we report on Raman scattering experiments on lead phthalocyanine (PbPc) layers (up to 20nm thick) deposited on GaAs(001) with c(4x4), (2x4) and (4x2) reconstructed surfaces. The Raman intensity selection rules of the PbPc vibrational modes are analyzed with respect to the GaAs(001) substrate coordinate system by rotating the sample around its normal. We find that some Raman intensities of the PbPc molecular vibratonal modes, depending on the initial surface reconstruction, vary with a period exactly correlated with the GaAs(001) substrate phonons modes. These findings prove an epitaxial growth mode of the PbPc layers on the GaAs(001) substrate. The results are in agreement with scanning tunneling microscopy (STM) results on submonolayer coverages demonstrating a correlation between the initial GaAs(001) surface structure and the PbPc layer properties.

DS 42.57 Wed 15:00 P1

Tailoring defect structure in nano porous alumina templates — •Hongdan Yan[1], Dirk Wulferding[1], Peter Lemmens[1], Jianmin Shi[2], Klaus Dieter Becker[2], Fatih Kalkan[3], Karina Morgenstern[3], Aidin Lak[4], and Meinhard Schilling[4] — [1]IPKM, TU-BS, Braunschweig, Germany — [2]IPTC, TU-BS, Braunschweig, Germany — [3]IFP, LU Hannover, Germany — [4]EMG, TU-BS, Braunschweig, Germany

Self organized, nanostructured materials are interesting from both fundamental and applied point of view. Often their optical properties are deteriorated by fluorescence due to oxygen defects. In the present study we demonstrate how preparation conditions and a consequent annealing can be used to optimize both morphology and defect structure of templates. These templates are used to realize plasmonic devices by a electrochemical deposition of Au wires.

Work supported by DFG, IGSM and NTH.

DS 42.58 Wed 15:00 P1

Optical and electrical properties of nano-Si embedded in silica as novel solar cell semiconductor — •David Friedrich, Karl-Heinz Heinig, and Bernd Schmidt — Helmholtz-Zentrum Dresden-Rossendorf (HZDR), Germany

Silicon photovoltaic (PV) modules are based on monocrystalline, microcrystalline or thin film amorphous silicon. Nanostructured Si might be one approach to achieve lower costs of electricity (€/Wp) by higher PV cell efficiency without substantial increase of fabrication costs.

Here we present measurements of optical and electrical properties of Si nanocrystals and sponge-like nano-Si morphologies embedded in silica. These Si nanostructures are fabricated by sputter deposition of SiOx followed by thermally activated nucleation or spinodal decomposition, resulting in Si nanoclusters or Si nanosponge, respectively. Due to the nanoscale feature size of the obtained Si sponge its band gap is opened by quantum confinement. Compared to separated Si nanoclusters, the spongy morphology ensures a higher electrical conductivity due to percolation.

Optical absorption, reflection and transmission data of SiOx and phase separated Si nanostructures will be presented for different compositions, i.e. x-dependent. The SiOx composition has been measured by Rutherford Backscattering (RBS). Additionally, spectroscopic ellipsometry and photolumiscence studies have been performed. These results will be discussed together with electrical resistivity measurements.

DS 42.59 Wed 15:00 P1

Local elemental and surface chemistry analysis of laser-nanostructured thin Au films — •Jürgen W. Gerlach, Marisa Mäder, Thomas Höche, Dietmar Hirsch, and Bernd Rauschenbach — Leibniz-Institut für Oberflächenmodifizierung, 04318 Leipzig

A regular arrangement of substrate-bound Au dots in fields of about 100 μm x 100 μm in size was obtained by structuring a thin Au film, which was deposited on a sapphire substrate, by Diffraction Mask Projection Laser Ablation (DiMPLA) [1]. Typical dot diameters of 150 nm to 200 nm resulted. Transmission electron microscopy revealed that during the structuring process with a single excimer laser pulse (KrF, 248 nm wavelength, 25 ns pulse length) the near-surface region of the single crystalline substrate melted and the Au dots were drawn partially or fully into the superficially molten substrate. Eventually, the Au dots were in parts embedded in the then amorphous near surface region of the substrate. In the present study, such fields of well-arranged Au dots on sapphire are investigated regarding the lateral elemental distribution as well as the surface chemistry by photoelectron spectroscopy. The results of elemental parallel imaging and small spot electron spectroscopy are compared with the actual distribution of Au dots in the structured fields as obtained by scanning electron microscopy. The presented results are discussed regarding localized charging effects or alternatively the formation of gold oxide. In the latter case, reaction of the Au dots with oxygen from the surrounding air during the laser structuring process has to be taken into account.

[1] M. Mäder et al., Phys. Stat. Sol. B, 247 (2010) 1372.

DS 42.60 Wed 15:00 P1

Mesostructured zinc oxide as basis material for dye-sensitized solar cells — •Christoph Richter[1], Michael Schröder[2], Bernd Smarsly[2], and Derck Schlettwein[1] — [1]Institute of Applied Physics, Justus-Liebig-University Giessen, Germany. email:schlettwein@uni-giessen.de — [2]Institute of Physical Chemistry, Justus-Liebig-University Giessen, Germany

Polysterene (PS) spheres of a narrow size distribution were synthesized by mini-emulsion polymerization. Films (1 - 10 μm) of densely packed PS spheres were prepared from suspensions of the spheres on fluorine-doped tin oxide films on a carrier substrate. Macroporous ZnO films were electrodeposited into the free space between the polystyrene spheres. The PS template was removed by solvent or UV treatment leaving behind the macroporous ZnO matrix. In a subsequent deposition step, additional ZnO was electrodeposited into the macropores this time, however, using a molecular template and hence forming mesoporous ZnO filling the space which ad been occupied by the PS spheres before. The films were characterized and their applicability as hierarchical structures in dye-sensitized solar cells will be discussed.

DS 42.61 Wed 15:00 P1

Piezoresponse force measurements on hetero-epitaxially grown Sodium-Bismuth-Titanate (NBT) thin films deposited by MOCVD-technique — •Andreas Duk, Jutta Schwarzkopf, Günter Wagner, Saud Bin Anooz, and Roberto Fornari — Institute for Crystal Growth, Berlin, Germany

Epitaxially grown Sodium-Bismuth-Titanate (NBT) thin films deposited by the MOCVD-technique on SrTiO3, NdGaO3 and DyScO3 were investigated by local piezoresponse force measurements. Aurivillius phases with m = 3, m= 3.5 and m = 4 and the Na0.5Bi0.5TiO3 perovskite phase were realized by varying the substrate temperature and/or the Na/Bi ratio in the gas phase. It has been observed that the effective piezoelectric coefficient increases with increasing number of perovskite units between two (Bi2O2)2+ intermediate layers. The influence of the lattice strain in the films on the piezoelectric response and the ferroelectric properties were studied by using different oxide substrates and films with variable film thickness.

DS 42.62 Wed 15:00 P1

Combined Quasi-Magnetoresistive Magnetic Field Sensor utilizing Magnetostriction and Quantum Tunneling — Bodo Henkel[1], Amit Kulkarni[1], •Thomas Strunskus[1], Vladimir Zaporojtchenko[1], Christoph Bechtold[2], Eckhard Quandt[2], and Franz Faupel[1] — [1]Multicomponent Materials, Institute for Materials Science, University of Kiel, Kaiserstr. 2, 24143 Kiel, Germany — [2]Inorganic Functional Materials, Institute for Materials Science, University of Kiel, Kaiserstr. 2, 24143 Kiel, Germany

A new concept of magnetic field sensor was developed and characterized. It uses the combination of magnetostriction provided by a Terfenol-D substrate and quantum tunneling through a 2D gold cluster array which is in the regime near to percolation threshold. There already a small magnetically induced elongation of the Terfenol-D crystal will lead to a well measurable change of current through the cluster array. An additional feature of the specific design of the sensor is direction sensitivity with regard to external magnetic fields. The sensor was characterized in terms of sensor signal hysteresis, sensitivity, repeatability, aging behaviour and the effect of cluster embedding into the underlying polymer layer. A well defined repeatable hysteresis with a change in signal amplitude (current) of 5.50 % was achieved in first experiments. Designs for higher ratios are in progress.

DS 42.63 Wed 15:00 P1

Nanocomposites prepared by plasma polymerization and cluster deposition — •Tilo Peter[1], Maike Wegner[1], Thomas Strunskus[1], Vladimir Zaporojtchenko[1], Sven Bornholdt[2], Holger Kersten[2], and Franz Faupel[1] — [1]Institute for Materials Science, Kiel, Germany — [2]Institute of Experimental and Applied Physics, Kiel, Germany

Recently, there is much interest in nanocomposites consisting of metal nanoparticles dispersed in a dielectric matrix due to their novel functional properties [1,2]. In many cases the formation of metal clusters is affected by chemical reactions with the host matrix material during deposition. The integration of a magnetron cluster source into a plasma deposition process allows the pre formation of clusters in the gas phase and subsequent codeposition with the matrix material. Here we focus on the properties of Ag clusters and the subsequently obtained nanocomposites by embedding in a polymer matrix which is deposited by plasma polymerization of Hexamethyldisiloxane. Two possible deposition systems are investigated: In the first system the cluster formation and plasma polymerization take place in the same plasma region, while in the second system the cluster formation takes place in a separate atmosphere and at different plasma parameters. The cluster and nanocomposite film properties were investigated by x-ray photoelectron spectroscopy, transmission electron microscopy and UV/Vis spectroscopy.

[1] Faupel,F. et.al., Contrib. Plasma Phys. 47(2007), 537.

[2] Faupel,F. et.al., Adv. Eng. Mater. (2010) accepted.

DS 42.64 Wed 15:00 P1

Customized arrangements of a-Ge nanocolumns by glancing angle deposition — •Jens Bauer, Michael Weise, Chinmay Khare, Christoph Grüner, and Bernd Rauschenbach — Leibniz-Institut für Oberflächenmodifizierung, Permoserstrasse 15, D-04318 Leipzig, Germany

We present PVD investigations on self-organized a-Ge nanostructures by glancing angle deposition (GLAD). In particular, a Ge particle beam provided by ion-beam sputtering is directed under a flat angle to the substrate (glancing angle $< 5°$). As a result of shadowing inclined nanoneedles evolve competitively. By use of substrate rotation the nanostructure can be customized to vertical posts, screws or spirals. To improve nanostructure arrangement and uniformity patterned substrates with symmetrically ordered surface mounds were applied: square and hcp orders by electron beam lithography and honeycomb or hcp orders by nanosphere lithography. The temporal evolution is distinguished by three morphological stages: 1) Initially the shape and size of the pre-pattern mounds determine the GLAD structures' shape. The structure thickness successively broadens. 2) Following a columnar shape with parallel border planes is obtained reflecting the pattern symmetry: square cross-section for square order, three-fold for honeycomb, and hexagonal to round for hcp. Characteristic caps are formed at the nanostructures' tops. Both the size of the border planes and the cap size depend strongly on the glancing angle and the pattern periodicity. 3) Caused by increasing competition the formation of individual GLAD columns stops and the pre-pattern arrangement gets lost.

DS 42.65 Wed 15:00 P1

Reflectivity characterization of silicon ion-implanted PMMA for device application at 1.55 μm — •Bojana Florian[1], Ivan Stefanov[2], and Georgi Hadjichristov[3] — [1]Bulgarian Institute of Metrology, 2 Prof. P. Mutafchiev Str., 1797 Sofia, Bulgaria — [2]Dept.of Quantum Electronics, Faculty of Physics, Sofia University, 5 James Bourchier Blvd., 1164 Sofia, Bulgaria — [3]Institute of Solid State Physics, 72 Tzarigradsko Chaussee Blvd., 1784 Sofia, Bulgaria

Silicon ion-implanted poly(methyl methacrylate) (PMMA) ultrathin layers of thickness of 100 nm buried in a depth of 100 nm were characterized by means of their near-IR reflectivity. As a case of photonic application for an integrated optics purpose (in optical devices operating at the telecommunications wavelength of 1.55 μm), we will present here an ultrathin reflective-type beam splitter/coupler with a low absorption loss. Such an optical element was examined upon illumination with the output of a 1.55 μm CW laser source coupled to an optic fiber.

Specular reflectance-to-transmission ratio (R/T) of PMMA plates implanted with Si+ ions at an energy of 50 keV and ion fluence in the range from 10^14 to 10^17 cm^2 were analyzed as a function of the ion-implant fluence, as well as the angle of incidence, polarization and the power of incident laser beam. Diffuse reflectivity of the layers at 1.55 μm was also carefuly measured. The nanoclustered structure of the carbonaceous subsurface ion-implanted layer enhances R/T [1].

[1] G.B. Hadjichristov, I.L. Stefanov, Appl. Opt. 49 (2010) 1876.

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DS 42.66 Wed 15:00 P1

Growth and optimization of YBa$_2$Cu$_3$O$_{7-x}$-SrTiO$_3$-

multilayers — •Alexander Guillaume, Frank Ludwig, Jan M. Scholtyssek, and Meinhard Schilling — Institut für Elektrische Messtechnik und Grundlagen der Elektrotechnik, Technische Universität Braunschweig, Hans-Sommer-Str. 66, D-38106 Braunschweig, Germany

$\mathrm{YBa_2Cu_3O_{7-x}}$ (YBCO) is a commonly used high-$\mathrm{T_c}$ superconducting material. Lattice matched insulating materials, such as $\mathrm{SrTiO_3}$ (STO), are required for the fabrication of complex multilayer devices. We grow STO-YBCO multilayers on (100)-surfaces of STO-substrates via pulsed laser deposition (PLD). Here, the optimization of the PLD-parameters for the deposition of YBCO by using the technique of design of experiments (DOE) based on [1] is presented. Another DOE for optimizing the parameters of the insulating STO-films is currently carried out. The parameters varied are the energy density of the laser pulses, the oxygen partial pressure inside the recipient and the temperature of the substrate. The optimization took into account the morphological, electrical and superconducting properties of the films. Atomic-force-micrographs are presented to illustrate the film morphology. Screening measurements were performed to investigate the superconducting transition characteristics and the homogeneity of the YBCO-layer while the van der Pauw-method was used to determine the thin film-resistivity.

[1] J.K. Heinsohn, D. Reimer, A. Richter, K.O. Subke, and M. Schilling, Physica C **299** (1998) 99-112.

DS 42.67 Wed 15:00 P1

Deposition of diamond-like carbon films on 3D substrates by liquid electrochemical technique — •Yangyang He[1], Guifeng Zhang[2], and Volker Buck[1] — [1]Thin Film Technology Group, Faculty of Physics, University Duisburg-Essen and CeNIDE, 47057, Duisburg, Germany — [2]School of Materials Science and Engineering, Dalian University of Technology, 116024, Dalian, China

Diamond-like carbon (DLC) films were simultaneously deposited on horizontally and vertically aligned stainless steel substrates by liquid electrochemical technique at low temperature. The applied potential and deposition time were 1000V and 2h. Isopropyl alcohol was chosen as electrolyte due to the advantages of high dielectric constant and small viscosity. SEM showed that the films deposited on horizontally aligned substrate were smooth and homogeneous. The films had uniform thickness on the whole surface of the horizontally aligned substrates. Raman analysis confirmed that typical DLC films were deposited on both substrates. The results showed that the films deposited on the horizontally aligned substrates had quite similar Raman spectra all over the surface. However, Raman spectra of the films deposited on the vertically aligned substrates appeared different depending on the position inside the solutions. The intensity of Raman spectra was supposed to correlate with the film thickness. It could be concluded that DLC films can be deposited on 3D substrates by liquid electrochemical technique which is of great importance in the industrial applications of DLC films.

DS 42.68 Wed 15:00 P1

Design and construction of an apparatus for the deposition of mass selected metal clusters — •Arne Fischer, Herbert Gleiter, and Horst Hahn — Karlsruher Institut für Technologie, Institut für Nanotechnologie, 76344 Eggenstein-Leopoldshafen, Germany

We report on the design and the construction of an apparatus for the non-destructive deposition of mass selected metal clusters. It will give us the opportunity to study clusters on various surfaces as well as clusters buried in matrices of other materials.

The clusters are provided by a magnetron sputter source installed in a liquid nitrogen cooled tube. The cold surrounding allows the sputtered atoms to condense to clusters, which are extracted by a helium stream. Depending on the mode of operation either anions or cations are accelerated and formed to an ion beam by electrostatic lenses. Downstream the beam gets mass separated in a 90° sector magnet (r = 500mm, resolution approx. 1/50), decelerated by an array of two einzellenses and finally soft landed on a cooled substrate (landing energy approx. 0.1 eV/atom). The matrix material can be optionally co-deposited via an integrated MBE.

DS 42.69 Wed 15:00 P1

Multiscale study of submonolayer growth for Fe/Mo(110) — •Martin Mašín[1], Mika O. Jahma[2], Tapio Ala-Nissila[2], and Miroslav Kotrla[1] — [1]Instute of Physics, Academy of Sciences of the Czech Republic, Na Slovance 2, Prague, 18221, Czech Republic — [2]Department of Applied Physics, Aalto University School of Science, P.O. Box 11000 , FI-00076 Aalto, Espoo, Finland

We apply a multiscale approach to study growth during Molecular Beam Epitaxy (MBE) in submonolayer coverages for Fe/Mo(110). We compare results obtained for island size distributions from two methods – the Kinetic Rate Equation (KRE) approach and Monte Carlo (MC) simulations. The relevant energy parameters in MC are the activation energy for single–particle jumps, binding energy to the substrate, and attractive adatom interactions. In the second part we use the KRE approach combined with the Particle Coalescence Method to compute the island size distributions. KRE gives time evolution of the island size distributions for a system undergoing diffusion driven aggregation. Incoming parameters are diffusion coefficients, obtained from independent MC simulations, and aggregation kernels. For comparison we use the scaled island density function $g(x)$ as a function of the normalized island size $x = s/\bar{s}$. In the case of KRE we use adatom–island and island–island aggregation modes at two temperatures 500 K and 1000 K. In the case of MC we consider only 500 K due to computational demands. At this temperature we have good agreement for the scaling function between the MC and KRE adatom–island aggregation models.

DS 42.70 Wed 15:00 P1

PCMO thin film for resistive switching devices — •Anja Herpers, Chanwoo Park, Tobias Menke, Rainer Bruchhaus, Regina Dittmann, and Rainer Waser — Peter Gruenberg Institute (PGI-7), Electronic Materials, Forschungszentrum Juelich, 52425 Juelich, Germany

In many transition metal oxides the electrical resistance can be changed between two defined values by applying an electrical field. This effect can be used in resistive random access memories for non-volatile data storage.

In this work the material $\mathrm{Pr_{0.48}Ca_{0.52}MnO_3}$ (PCMO) as perovskite oxide and its interface to titanium and platinum is investigated. For the thin film preparation RHEED-assisted pulsed laser deposition is used. The material is epitaxially grown on $\mathrm{SrTiO_3}$ substrates and $\mathrm{SrRuO_3}$ films under different conditions. The deposition parameters have been optimized in regard of RHEED pattern (50 unit cell layers visible), surface roughness down to 2Å by AFM and crystal quality using XRD (FWHM of rocking curve down to 0.034°). We will compare devices having interfaces to metals with different work functions, as it is considered in literature that the Schottky barrier is changed during switching. We will present the corresponding I-V-curves and switching results.

DS 42.71 Wed 15:00 P1

Investigations of Thin Films Derived from Nanocrystalline Silicon Powder applying Raman, Infrared Spectroscopy, and Spectroscopic Ellipsometry — •Falko Seidel[1], Ovidiu D. Gordan[1], Roy Buschbeck[2], Alexander Jakob[2], and Dietrich R. T. Zahn[1] — [1]Semiconductor Physics, Chemnitz University of Technology, D-09107 Chemnitz, Germany — [2]Inorganic Chemistry, Chemnitz University of Technology, D-09107 Chemnitz, Germany

Thin film solar cells can have the advantage of being mechanically flexible and at the same time reducing material and production costs. At present, two main types of photovoltaic (PV) cells are found marketing applications: II-VI respectively II-III-VI compound semiconductors (CdTe, Cu(In,Ga)(S,Se)2 CIGS) and amorphous silicon (a-Si). The optical band gap of non-silicon CIGS PV cells can be tuned by changing the ratio of the incorporated elements. The most important advantage of Si is its availability. For application in solar cells it would be desirable to tune silicon properties as well. Thus, nanocrystalline silicon (nc-Si) is of great interest because of the band gap being tuneable with the particle size. The confinement effect leads to a shift of the optical band gap to higher energies. Additionally, the use of nanocrystalline powder makes price-efficient printing processes in the production feasible.

In this work optical characterisation of nc-Si powder and drop coated nc-Si films is presented using Raman Spectroscopy, Fourier Transform Infrared Spectroscopy (FTIRS), and Variable Angle Spectroscopic Ellipsometry (VASE).

DS 42.72 Wed 15:00 P1

Magneto-optical Kerr effect studies of copper oxide and cobalt thin films — •Michael Fronk[1], Steve Müller[2], Thomas Waechtler[2], Stefan E. Schulz[2], Dietrich R.T. Zahn[1], and Georgeta Salvan[1] — [1]Chemnitz University of Technology, Chemnitz, Germany — [2]Fraunhofer Research Institution for Electronic Nano Systems ENAS, Chemnitz, Germany

Copper oxide is supposed to be a model material for tunnel-magneto-resistance (TMR) structures together with cobalt as ferromagnetic electrode. Therefore the magnetic properties of copper oxide itself are of interest and under investigation by various techniques. This contribution will present spectroscopic magneto-optical Kerr effect (MOKE) studies of thin films of this material. The films are produced by atomic layer deposition based on a Cu(I) β-diketonate precursor at a process temperature of 120°C. The copper oxide films turned out to be magneto-optically active both in the spectral range around 2 eV and above 4 eV. Besides the experimental MOKE data the material-intrinsic magneto-optical Voigt constant extracted from optical model calculations will be presented. Cobalt, the ferromagnetic counterpart in the TMR structures, was prepared by magnetron sputtering as thin films with different thicknesses. The Voigt constant of Co can be deduced from measurements on thick films (˜ 120 nm). It is investigated whether these data can be used to predict the magneto-optical response of thinner Co layers (˜ 10 nm).

DS 42.73 Wed 15:00 P1

Deep Trap Analysis using QTS and DLTS on Schottky Diodes with Gold Implanted Silicon — •Markus Arnold, Axel Fechner, Susann Müller, and Dietrich R.T. Zahn — Chemnitz University of Technology, Semiconductor Physics, 09107 Chemnitz, Germany

Charge transient spectroscopy (QTS) and deep-level transient spectroscopy (DLTS) measurements of Silicon Schottky diodes are presented revealing the influence of gold implantation into n-doped silicon on the charge carrier transport and trapping properties.

Charge transient spectroscopy (QTS) developed originally by Kirov et al. [1] is an electrical measurement method related to deep-level transient spectroscopy (DLTS) developed originally by Lang et al. [2]. Especially using QTS it is possible to measure high ohmic structures like Metal-Oxide-Semiconductor (MOS) capacitors with a high sensitivity. Due to the leakage current in the reverse bias region of Schottky diodes it is very challenging to measure QTS. So the results obtained using QTS are compared to current-voltage, capacitance-voltage, and DLTS measurements on the same samples. The compatibility of these techniques and their differences are discussed.

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[2] D. V. Lang, J. Appl. Phys. 45 (1974) 3023

DS 42.74 Wed 15:00 P1

Spectroscopic Investigations of DC Magnetron Sputtered Amorphous Silicon Thin Films — •Philipp Schäfer[1], Frank Nobis[2], Markus Arnold[1], Ovidiu D. Gordan[1], Hartmut Kupfer[2], Frank Richter[2], and Dietrich R. T. Zahn[1] — [1]Semiconductor Physics, Chemnitz University of Technology — [2]Solid State Physics, Chemnitz University of Technology

Spectroscopic techniques were used to provide an in-depth analysis of dc magnetron sputtered hydrogenated amorphous silicon (a-Si:H) layers for photovoltaic applications. The complex optical dispersion in the range from 0.7 eV to 5.0 eV was determined using variable angle spectroscopic ellipsometry. A shift of the absorption onset to higher energies for samples sputtered at increased hydrogen flow rates is related to less defect states within the mobility gap. In order to calculate the hydrogen content of the deposited layers, the absorption due to silicon-hydrogen stretching vibrations was evaluated employing Fourier transformed infrared (FTIR) spectroscopy. A linear relationship between the absorption onset and the hydrogen concentration is observed. Raman spectroscopy confirms the purely amorphous nature of the silicon network. A deeper understanding of the states within the mobility gap is obtained from electrical spectroscopic techniques. Charge deep level transient spectroscopy measurements at various temperatures probe the defect level energy and concentration. Furthermore, a comparison with densities estimated by drive level capacitance profiling is provided.

DS 42.75 Wed 15:00 P1

Mechanical dissipation in thermally grown silica at low temperatures — •Julius Komma[1], Christian Schwarz[1], Gerd Hofmann[1], Daniel Heinert[1], Ronny Nawrodt[1], Giles Hammond[2], and Paul Seidel[1] — [1]Friedrich-Schiller-Universität Jena, Institut für Festkörperphysik, Helmholtzweg 5, D-07743 Jena, Germany — [2]Glasgow University, G12 8QQ Glasgow, UK

Silica (SiO_2) is a common material as low index material in thin optical layers. Its mechanical loss is of great interest since the thermal noise of a surface layer is directly related to its mechanical loss by means of the fluctuation dissipation theorem. It is well known that bulk silica shows a very large dissipation peak at cryogenic temperatures between 30 and 40 K.

We present a detailed analysis of the mechanical loss of thin silica layers with a thickness between 0.1 and 3 μm in a temperature range from 5 to 300 K. The measurements have been performed in a ring-down technique. The layers have been produced by thermal oxidation of thin silicon flexures.

The dependence of the mechanical loss of the layer thickness is discussed and a possible transition of the micro-structure from a thin layer to a thick layer model is presented. The comparison of the activation energy of the dissipation process reveals differences between the bulk silica and thin layer silica samples.

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DS 42.76 Wed 15:00 P1

Enhancement of growth and structure properties of $YBa_2Cu_3O_{7-\delta}$ thin layers by in situ incorporation of gold nano-clusters — •Ralf Erlebach[1], Michael Hübner[1], Sandra Christke[1], Veit Grosse[1], Frank Schmidl[1], Jürgen Kräusslich[2], Markus Rettenmayr[3], and Paul Seidel[1] — [1]Friedrich-Schiller-University Jena, Institute of Solid State Physics, Helmholtzweg 5, 07743 Jena, Germany — [2]Friedrich-Schiller-University Jena, Institute of Optics and Quantum Electronics, Max-Wien-Platz 1, 07743 Jena, Germany — [3]Friedrich-Schiller-University Jena, Institute of Materials Sciene and Technology, Löbdergraben 32, 07743 Jena, Germany

For most hetero-epitactic growth techniques, structural defects due to the lattice misfit, namely tilts, precipitates or holes, turn out to be limiting factors for the succesful fabrication of multilayer systems. A new approach of an in situ growth technique dealing with this problem by incorporation of gold nano-clusters is examined. Therefore, pulsed laser deposition (PLD) of a high-T_C $YBa_2Cu_3O_{7-\delta}$ (YBCO) layer onto a strontium titanate (STO) template with a temporary interlayer of gold with a well-defined film thickness is investigated. Within this process, the gold interlayer shows nano-clustering behavior.

Effects on the properties of structure like crystallographic or surface features of the ablated YBCO layer by variation of the film thickness of the gold and YBCO layers are presented. Moreover, distribution and clustering behavior of the crystallized gold nano-particles as well as the basic superconducting properties of the layer system are analyzed.

DS 42.77 Wed 15:00 P1

Investigation of improvements of electrical and optical properties of reactively sputtered ZnO:Al thin films upon post-deposition thermal annealing — •Patrick Ries, Dominik Köhl, and Matthias Wuttig — I. Institute of Physics (IA), RWTH Aachen University, 52056 Aachen, Germany

Aluminium-doped zinc oxide (ZnO:Al) has gained significant scientific and industrial interest during the past decade. Particularly, ZnO:Al films have become the material of choice in the fabrication of transparent electrodes for silicon thin film solar cells, which offer a low-cost alternative to wafer-based highly-efficient but more expensive modules. ZnO:Al films exhibit high optical transparency. The electrical conductivity is only by a factor of 3 smaller than the one of ITO films. ITO is the most commonly used but more expensive Transparent Conducting Oxide. Consequently, efforts are presently focused on improving film properties to improve the electrical conductivity of ZnO:Al to potentially replace ITO in the near future. To accomplish this goal, post-deposition annealing of the specimens to cure defects is investigated in the present study. The aim is to thoroughly understand the principle scattering mechanisms. The electrical and optical properties as a function of annealing temperature are investigated by Ellipsometry, FTIR & UV/VIS spectroscopy, van der Pauw and Hall measurements. Conclusions on the dominant scattering channels and their temperature dependence are drawn.

DS 42.78 Wed 15:00 P1

Photocatalysis in sputtered TiO_2 thin films: Measurement of the surface work function to correlate structural features with photocatalytic activity — •Alexandra Yatim, Dominik Köhl, and Matthias Wuttig — I. Physikalisches Institut IA, RWTH Aachen, Germany

Titanium dioxide (TiO_2) is known for its very unique physical properties. Specifically, TiO$_2$ provides a large refractive index and a pronounced photocatalytic activity. Therefore it has become the material of choice in the fabrication of anti-reflective or self-cleaning coatings in architectural glazing. Interestingly, although products already exist on the market, little is known about the underlying mechanism governing the strong photocatalysis. This particularly includes insufficient knowledge about the influence of the specific coating process on the activity of the films. In the architectural glazing industry, magnetron sputtering is preferably utilized since it provides both, homogeneity of the coating on large area substrates and flexibility in the choice of materials. Hence, it is the aim of the present work to investigate the photocatalytic properties of sputtered TiO$_2$ thin films. Kelvin Probe measurements to determine the surface photovoltage of the specimens under UV illumination are utilized. The data is compared and correlated with data of structural properties from XRD and AFM measurements and with the specific deposition conditions. The major goal of the study is to explain the photocatalytic activity of the specimens on a microscopic scale and hence to find criteria that allow for the fabrication of highly active coatings.

DS 42.79 Wed 15:00 P1

Improved lateral conductivity of a two phase SiO:ucSi[n] intermediate reflective layer in thin film solar cells — Burkhard Gilles[1], Ulrich Heinzmann[1], Helmut Stiebig[2], Stefan Gruss[2], and •Florian Maier[2] — [1]Univ. of Bielefeld, Faculty of Physics, Molecular & Surface Physics — [2]Malibu GmbH Co. KG

Increasing the efficiency of thin film solar cells is a crucial requirement for competing with other technologies in the field of solar energy conversion. After the introduction of thin film tandem solar cells, light management has become an important issue to achieve this end. The application of intermediate reflective layers is a promising approach for the optimisation of the light distribution between top and bottom cell. Numerous works on this field have been carried out so far. However, a major problem is the poor conductivity of those films which lead to an increase of the series resistance. The application of a layer of doped silicon oxide containing a phase of microcrystalline silicon (μc-SiOx:H <n>) can overcome this problem. The experiments were carried out on samples of industrial scale (1.1 m x 1.3 m). A number of possibilities for the suppression of the lateral resistivity have been examined. A substantial increase of conductivity has been achieved. The correlation of growth conditions, thickness and conductivity will be discussed.

DS 42.80 Wed 15:00 P1

Thin SiO films condensed at different substrate temperatures studied by infrared spectroscopy — •Steffen Wetzel[1], Hans-Peter Gail[2], and Annemarie Pucci[1] — [1]Kirchhoff-Institut für Physik, INF 227, 69120 Heidelberg — [2]Institut für Theoretische Astrophysik, Albert-Ueberle-Str. 2, 69120 Heidelberg

Silicon oxides are not only of basic scientific interest but also of great importance in microelectronics and of considerable relevance in astronomy as building blocks of silicates, the most abundant minerals in space. Their spectral features can reveal the chemical composition and inform on formation conditions as gas pressure or temperature. To look into the origin of IR spectral changes, the growth of thermally evaporated silicon monoxide (SiO) on silicon substrates was studied in situ by infrared spectroscopy under ultra-high vacuum conditions. Previous studies on the growth of ultrathin films on clean Si(111) showed a thickness dependent shift of the main vibrational line of up to 120 cm^{-1} compared to the bulk value of 984 cm^{-1} [1, 2] at 300 K substrate temperature. In our recent study we investigated the influence of different substrate temperatures on the condensation process. Measurements at temperatures between 40 K and 500 K reveal a clear shift of the vibrational peak position from 960 cm^{-1} to 1000 cm^{-1} with increasing temperature. Details on the experimental setup and explanations for the observed peak shift will be presented.

[1] M. Klevenz et al. Phys. Status Solidi B, 247(9), 2179-2184 (2010)

[2] M. Klevenz et al. Applied Spectroscopy, 64(3), 298-303 (2010)

DS 42.81 Wed 15:00 P1

The effect of gold nanoclusters on the growth and properties of homoepitaxial strontium titanate layers — •Sandra Christke[1], Ralf Erlebach[1], Frank Schmidl[1], Jürgen Kräusslich[2], Markus Rettenmayr[3], and Paul Seidel[1] — [1]Friedrich-Schiller-University Jena, Institute of Solid State Physics, Helmholtzweg 5, 07743 Jena, Germany — [2]Friedrich-Schiller-University Jena, Institute of Optics and Quantum Electronics, Max-Wien-Platz 1, 07743 Jena, Germany — [3]Friedrich-Schiller-University Jena, Institute of Materials Science and Technology, Löbdergraben 32, 07743 Jena, Germany

We use pulsed layer deposition (PLD) to fabricate single crystal thin films and layer systems which can be epitaxially deposited. Here we present analysis regarding the growth of strontium titanate (STO) layers on single crystal STO substrates. The specific characteristic of these experiments is the deposition of the STO layer through PLD. Therefore, during the formation of the STO layer onto the substrate the initial gold layer is transformed into nanoclusters. We show the dependence of crystallographic and optical properties as a function of gold and STO layer thicknesses as well as surface parameters.

DS 42.82 Wed 15:00 P1

Investigation of optical and electrical properties of magnetron sputtered ZnO:Al films for in-line characterization — •Regina Nowak, Benedikt Schumacher, Daniela Rogler, Karsten von Maydell, and Carsten Agert — NEXT ENERGY, EWE-Forschungszentrum für Energietechnologie e.V.

Due to cheaper and easier processing, thin film solar cells promise a substantial cost reduction potential compared to conventional crystalline silicon solar cells. The front electrode of these devices consists of a transparent conducting oxide (TCO) layer. In the case of hydrogenated amorphous (a-Si:H) and microcrystalline (μc-Si:H) silicon thin film solar cells, aluminum doped zinc oxide (ZnO:Al) is widely used as TCO.

In this study, the influence of the variation of the process parameters on the optical and electrical properties of ZnO:Al has been analyzed. Therefore ZnO:Al layers on glass were deposited under varying conditions using magnetron sputtering. The ZnO:Al films were characterized by spectroscopic ellipsometry, raman spectroscopy, four-point probe and AFM. The aim of these investigations is to find measurable values which can be used for cheap process control. This shall later on be involved in an in-line characterization of the whole solar cell.

DS 42.83 Wed 15:00 P1

Significant stress reduction of cBN layers upon ion irradiation at elevated temperatures — •Stefan Weidner[1], Sebastian Geburt[1], Jian Ye[2], Sven Ulrich[2], and Carsten Ronning[1] — [1]Institut für Festkörperphysik, Friedrich-Schiller-Universität Jena — [2]Institut für Materialforschung, Forschungszentrum Karlsruhe

Cubic boron nitride (cBN) is the hardest materials beneath diamond and exceeds the properties in terms of chemical resistivity, making it a promising candidate for ultra-hard coatings in extreme environments. Due to the ion assisted growth process, the cBN layers suffer from an intrinsic stress, which limits the layer thickness and therefore possible industrial applications.

To investigate new approaches for the synthesis of low stress cBN layers, we applied ion irradiation with various ion species (O, Ne, Kr) and at different temperatures between 300 to 600 K to cBN:O layers [1]. The intrinsic stress and the cBN content were monitored by profilometer and FTIR after each implantation step. As expected, ion irradiation at room temperature leads to a stress reduction with constant cBN content upon an ion induced damage up to 0.5 dpa [2], but a severe damage is introduced to the layer above this value resulting into a phase transition to hBN. However, irradiation at elevated temperatures results in a significant stress reduction without decrease of the cBN quality even up to 4.3 dpa.

[1] Ye at al. Thin Solid Films 517(3), 2008, p.1151-1155

[2] Widmayer et al., Diamond and Related Materials 6, 1997, p. 621-625

DS 42.84 Wed 15:00 P1

Interdiffusion and Magnetic Properties of Buried Fe-Layers in Planar Cavities Containing C-matrix — •Balaram Sahoo[1], Ralf Roehlsberger[1], Kai Schlage[1], Ulrich von Hoersten[2], Werner Keune[2], Heiko Wende[2], Hans-Christian Wille[1], Wolfgang Calibe[1], Joern Donges[1], Roman Chernikov[1], Edmund Welter[1], and Andre Rothkirch[1] — [1]Deutsches Elektronen Synchrotron DESY, Notkestr. 85, 22607, Hamburg, Germany — [2]Universität Duisburg-Essen, Lotharstr. 1, D-47048 Duisburg, Germany

We report on the preparation of planar wave guides by DC magnetron sputtering with buried 57Fe-probe layers of varied thickness and the characterization of their interfaces and magnetism via X-ray diffraction (XRD), X-ray reflectivity (XRR), extended X-ray absorption fine structure (EXAFS) spectroscopy and 57Fe conversion-electron Mössbauer spectroscopy (CEMS). XRD, EXAFS and CEMS results suggests the amorphous nature of the diffused interface. CEMS results demonstrate that the Fe layers are paramagnetic at RT, when the Fe layer thickness was below 1.1 nm. A paramagnetic to ferromagnetic phase transition has been observed for increasing Fe layer thicknesses. In addition, intermixing between Fe and C atoms at the interfacial region has been observed as a distribution of magnetic hyperfine field in the CEM spectrum. The intermixing was estimated to be extended to about 1.2 nm on either side of the Fe layers; however, this is expected to be strongly dependent on the preparation method.

DS 42.85 Wed 15:00 P1

Characterization of lattice defects by X-ray absorption spectroscopy in ferromagnetic pure ZnO films — •Jörg Haug[1], Angelika Chassé[1], Stephan Borek[1], Manfred Dubiel[1], Muhammad Khalid[2], and Pablo Esquinazi[2] — [1]Department of Physics, University of Halle-Wittenberg, Von-Danckelmann-Platz 3, D-06120 Halle — [2]Division of Superconductivity and Magnetism, University of Leipzig, D-04103 Leipzig

ZnO films were grown on graphite substrates by pulsed laser deposition under different nitrogen pressure (0.01 - 1.0 mbar) using a KrF excimer laser. The film thickness was between 60 and 500 nm. X-ray diffraction experiments of (100) and (112) reflections demonstrate the a-plane orientation of pure ZnO films. The line broadening of reflection peaks yield crystallite sizes of approximately 50 nm. The comparison of XRD lattice parameters and Zn-O and Zn-Zn distances as determined by EXAFS experiments at the Zn K edge indicates a mismatch to the structure of ZnO single crystals as well as a slight dependence on nitrogen pressure. X-ray absorption experiments of the near edge region (XANES) show an orientation dependence of signals on x-ray polarization and a correlation between the intensity of 1s to 4p transition with the defect concentration. XANES simulations of Zn K edge by means of a multiple-scattering approach demonstrate the sensitivity to vacancy defects. With that structural models of defect centers has been developed to interpret the experimental data.

DS 42.86 Wed 15:00 P1

Picosecond-Pulsed Laser Deposition of $Ge_2Sb_2Te_5$ — •Julia Benke, Erik Thelander, and Bernd Rauschenbach — Leibniz Institute of Surface Modification, Leipzig

The chalcogenide compound $Ge_2Sb_2Te_5$ (GST) is a commonly used material for phase change applications like PC-RAM and optical data storage [1]. Here, we present thin films of GST synthesized by Pulsed Laser Deposition (PLD) using a picosecond laser. The use of ultrashort pulses drastically changes the ablation mechanism compared to conventional PLD and hence another type of film morphology is to be expected [2]. Samples have been deposited on glass and SiO_2 in an UHV-chamber in different inert gas environments. The influence of substrate temperature and target-to-substrate distance on the surface topography has been investigated and characterized with SEM and AFM whereas structural information has been obtained with XRD, XPS and RBS.

[1] Raoux S., Annu. Rev. Mater. Res., **48**, (2009), 39:25
[2] Teghil et al., Appl. Surf. Sci., **210** (2003), 307

DS 42.87 Wed 15:00 P1

Ultimate soft x-ray microspectroscopy for chemical analysis — •Andreas Späth[1], Jörg Raabe[2], Christian Hub[1], Stephan Wenzel[1], Benjamin Watts[2], and Rainer H. Fink[1] — [1]Friedrich-Alexander Universität Erlangen-Nürnberg, Physikalische Chemie II and ICMM, Erlangen, Germany — [2]Swiss Light Source (SLS), Paul Scherrer Institut, Villigen, Switzerland

Zone-plate based x-ray microscopes offer a wide range of potential applications in fundamental and applied science, in physics, chemistry and material science or in the imaging of biosamples. The present PolLux scanning transmission x-ray microspectroscope is installed at a bending magnet beamline of the Swiss Light Source (SLS) operating from 260 - 1200 eV [1]. Using the latest zone-plate technology, imaging of lateral structures with 12 nm periods was achieved [2]. The available energy range is ideally suited for soft matter investigations. We will present spectromicroscopic results from various organic based materials, like organic hybrid materials, polymer films, organic nanocrystals or biosamples. The recent extension of the detection setup by an electron multiplier offers additional surface-enhanced detection. Thus, we are able to combine bulk and surface sensitivity. In addition, differential phase-contrast imaging offers another detection scheme to improve image contrast. The complementary use of the various detection schemes offers improved knowledge on the investigated soft matter samples. The project is funded by the BMBF under contract 05 KS7WE1.

1. J. Raabe, et al., Rev. Sci. Instrum. 79, 2008, 113704.
2. K. Jefimovs, et al., Phys. Rev. Lett. 99, 2007, 264801.

DS 42.88 Wed 15:00 P1

Mechanical properties of thin sputtered a-C and CNx multilayers on polymer substrates — •Zdenek Stryhal[1], Martin Dubau[1], Arndt Schumann[1], Dieter Schneider[2], and Frank Richter[1] — [1]Chemnitz University of Technology,Reichenhainer Straße 70, D-09126 Chemnitz, Germany — [2]Fraunhofer IWS Dresden, Winterbergstrasse 28, 01277 Dresden, Germany

The aim of this work was to investigate the formation of carbonaceous layers on polymer substrates and to characterize the friction and wear behavior of those layers. Amorphous (nearly hydrogen free) carbon and nitrogen doped carbon films have been grown by pulsed DC magnetron sputtering from a graphite target in argon and argon/nitrogen gas mixture. Single films of these two materials as well as multilayers composed of them have been investigated. Our layer were deposited on various polymer substrates (polybutylene terephthalate – PBT and polyamide – PA66) that are used in industrial conveying systems. Following methods have been used to characterize deposited layers: stylus profilometer (intrinsic stress, compressive 0.1–5.5GPa), adhesion (pull-out test, >14MPa), reciprocating tribometer (wear resistance and friction coefficient, μ=0.15–0.35), bending test(deformation resistance), SAW (elastic modulus, 50–250GPa) and SEM (surface topography). Friction and wear tests were made at conditions similar to those we expect in real transport systems.

DS 42.89 Wed 15:00 P1

Resonant Photoelectron Spectroscopy of epitaxial Fe-doped $SrTiO_3$ — •Annemarie Köhl[1], Christian Lenser[1], Jacek Szade[2], Dariusz Kajewski[2], Jurek Kubacki[2], Regina Dittmann[1], Kristof Szot[1], and Rainer Waser[1] — [1]Peter Grünberg Institut (PGI-7), Forschungszentrum Jülich, Germany — [2]A.Chelkowski Institute of Physics, University of Silesia, Katowice, Poland

In recent years resistive switching in transition metal oxides received a lot of research interest due to the proposed application as non-volatile data memory. $SrTiO_3$ serves as a model system for investigation of resistive switching due to the valency change mechanism. Frequently slightly Fe doping is used, as it has shown to improve the switching properties.

Therefore the electronic structure of epitaxial Fe-doped $SrTiO_3$ was studied by photoelectron spectroscopy. Thin film samples with Fe concentration of 1 at.% and 2 at.% as well as undoped references are prepared by pulsed laser deposition and checked for surface quality by AFM. Core-level photoelectron peaks are analysed regarding the chemical shift and valence state. Resonant photoelectron spectroscopy at the absorption edge of Ti, O and Fe was used to determine the spectral contributions to the valence band. Most noteworthy we find significant spectral weight above the valence band, which can be attributed to Fe-states.

DS 42.90 Wed 15:00 P1

Influence of growth conditions on the crystallization behaviour of reactively magnetron sputtered amorphous molybdenum oxide films — •Sven C. Liepertz, Gomathi Natarajan, Dominik Köhl, Peter Zalden, and Matthias Wuttig — Institute of Physics IA, RWTH Aachen University

The objective of the present work is the synthesis and characterization of meta-stable crystalline phases of group IV and VI transition metal oxides. To grow such specimen, amorphous films are deposited by reactive magnetron sputtering of the elemental transition metal target. Crystallization is induced by thermal annealing and studied by XRD (phase information), SEM and optical microscopy (morphology). Special emphasis is put on the influence of specific features of the amorphous matrix on the crystallization behaviour. Particularly, the stoichiometry of the precursor is tailored by adjusting the deposition process parameters. The elemental composition of such specimen is deduced from RBS measurements. The optical properties of amorphous and crystalline films are investigated by spectroscopic ellipsometry and reflections/transmittance measurements in the UV/VIS spectral region. The optical data is modelled to determine the dielectric function which has been related to the crystallization behaviour.

The focus of the present study is on the investigation of MoO_3 films. It will be shown that films with different crystallization behaviour and corresponding crystalline phases can be fabricated by tailoring film deposition and subsequent annealing.

DS 42.91 Wed 15:00 P1

H_2 plasma modification of polydimethylsiloxane thin films investigated by infrared reflection absorption spectroscopy — •Vladimir Danilov, Hans-Erich Wagner, and Jürgen Meichsner — Ernst Moritz Arndt University of Greifswald, Germany

Plasma modification of polydimethylsiloxane (PDMS) thin films was studied by means of Fourier-Transform-Infrared-Reflection-Absorption-Spectroscopy. The spin-coated PDMS films with the thickness between 10 nm and 400 nm were prepared on Al-coated glass substrates and were treated by direct contact with H_2 plasma as well as by the H_2 plasma radiation, only. In direct plasma treatment the substrates were positioned on the powered electrode of an asymmetric capacitively coupled RF discharge in H_2 at low pressure. The influence of the plasma radiation was studied in different spectral ranges due to the screening of the thin film from the bulk plasma by selected window characterized by different cut-off wavelength: soda-lime glass (300 nm), quartz glass (160 nm) and MgF_2 (115 nm). The strong modification effect was observed in experiments with the MgF_2 window, only. The evolution of IR spectra was monitored, and the changes of PDMS characteristic absorption bands as well as the formation of new bands are discussed. It was found that the films consist of methyl-free SiO_x top layer (10-30 nm), followed by partially methyl-free region, and an underlying non-modified PDMS layer in the case of thin films prepared with initial thickness exceeding 350-400 nm.

Funded by the Volkswagen Foundation, Plasma Hybrid Coating, grant no. I/83275.

DS 42.92 Wed 15:00 P1

Low Energy SEM - High Resolution, Low Charging, Low Damage — •Philipp Tonndorf, Steffen Schulze, and Michael Hietschold — Chemnitz University of Technology, Reichenhainer Straße 70, D-09126 Chemnitz, Germany

With the usage of slow primary electrons in the scanning electron microscope it is possible to achieve more valueable images with respect to resolution, charging and damage. The primary electrons are accelerated as usual with some kV. Then after the last lens they are slowed down to some hundreds of eV through an opposing field. So the interaction volume shrinks and one gets higher resolution and better signal-noise-ratio. Another effect is a higher surface sensitivity. Through the smaller landing energy the SE and BSE yield changes. If the total yield is 1 no charging occurs. So it is possible to investigate insulators with no metal coating. With very slow primary electrons (< 50 eV) the damaging of organics and the carbon contamination decreases. At about 25 eV there is no more damage observed through ionisation. At this energy backscattering becomes inversely proportional to the local density of states. Carbon contamination stops at about 4 eV.

DS 42.93 Wed 15:00 P1

Trends in crystallization behavior of phase-change materials under high external pressure — •Matthias Kaes[1], Peter Zalden[1], Julia van Eijk[1], Giuliana Aquilanti[2], Sakura Pascarelli[2], and Matthias Wuttig[1] — [1]I. Physikalisches Institut (1A), RWTH Aachen University, D-52056 Aachen, Germany — [2]European Synchrotron Radiation Facility, Grenoble, France

Phase-change materials (PCMs) exhibit a rapid crystallization of their amorphous phase and a related change in electrical conductivity of several orders of magnitude. There have been estimations that high pressures (6 GPa) might occur in a phase-change random access memory (PCRAM)-cell due to thermal expansion, which could influence the switching mechanism in small PCRAM-cells. Moreover, PCMs show surprising pressure-dependent behavior, as the prototypical PCM $Ge_2Sb_2Te_5$ has been observed to amorphize under increasing pressures (10-20 GPa) [1].

Here, we present in-situ EXAFS experiments at the Ge K absorption edge by which we have investigated the pressure-induced changes in short-range order in $Ge_2Sb_2Te_5$ and $Ge_4Sb_1Te_5$.

While both materials show similar crystallization behavior under ambient pressure, it is found that the crystallization is influenced or even suppressed by applied external pressures. We compare our results with previous findings and derive stoichiometric trends, from which we propose that the reliability of PCRAM-devices could benefit from the use of PCMs with high content of GeTe.

[1] A.V. Kolobov et al. Physical Review Letters 035701, p. 2-5 (2006).

DS 42.94 Wed 15:00 P1

Preparation and X-Ray standing Wave Measurements of STO/LAO films — •Christoph Schlueter and Jörg Zegenhagen — ESRF, 6 rue Jules Horowitz, BP 220, 38043 Grenoble, CEDEX 9, France

The formation of a quasi-2dimensional electron gas at the interface of $SrTiO_3$ (STO) and $LaAlO_3$ (LAO) attracted considerable attention in recent years.[1] A X-ray standing wave (XSW) and X-Ray Photoelectron Spectroscopy (XPS) experiment is expected to help elucidate details of the electronic and atomic structure at the interface. Samples of high crystallographic quality are needed for these experiments. Samples were grown on (001) oriented STO single crystal substrates. TiO_2 termination was obtained by standard methods.[2] The thin films were deposited in a UHV compatible pulsed laser deposition (PLD) chamber using a UV laser (λ=248nm) at sample temperatures of 750 - 820°C in an oxygen atmosphere of $5*10^{-5}$ mbar. For samples held at elevated temperatures for longer times (tempering and/or slow cooling rate) steps were found to bunch by atomic force microscopy (AFM). This is indicative on a significant surface diffusivity at these temperatures. Faster cooling times (1-1.5h) resulted in smooth surfaces with unit cell height steps. AFM and reflectivity data are in reasonable agreement. For even higher cooling rates powder rings prove that parts of the film are badly oriented. Diffraction and XSW experiments indicate the formation of fully strained films.

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2. G. Koster et al., Appl. Phys. Lett. 73, no. 20 (1998): 2920-2922.

DS 42.95 Wed 15:00 P1

Anisotropic structural and electrical properties of strained SrTiO3 films on sapphire — •Thomas Grellmann, Kyrylo Greben, Eugen Hollmann, Rolf Kutzner, and Roger Wördenweber — Institute of Bio- and Nanosystems (IBN), Forschungszentrum Jülich, D-52425 Jülich

The electronic properties of oxide films strongly depend on the composition, structure and structural imperfections. Since lattice constants and thermal expansion coefficient of substrate and films are usually different, mechanical strain is imposed on the growing films. In this work we examine the strain of epitaxially grown SrTiO3 films on sapphire and its impact on the ferroelectric properties of the film. The lattice mismatch of about 10% between SrTiO3 and sapphire is reduced via a buffer layer, CeO2. The strain induced modification of the structure is determined via XRD measurements. High-resolution Pole-figure measurements demonstrate the anisotropic and thickness dependent (i.e., relaxation) distortion of the SrTiO3 lattice. Electronic characterization of the dielectric properties reveal the resulting anisotropy of the polarizability of film. Furthermore, it demonstrates that ferroelectric can be induced via strain in the originally incipient ferroelectric SrTiO3 up to high temperatures well above 200K.

DS 42.96 Wed 15:00 P1

In-Situ SEM Investigation Of Swift Heavy Ion Induced Dewetting — •Daniel Garmatter, Michael Haag, Redi Ferhati, Sankarakumar Amirthapandian, and Wolfgang Bolse — Institut für Halbleiteroptik und Funktionelle Grenzflächen, Universität Stuttgart

Recently we have found that swift heavy ion (SHI) irradiation of thin oxide films on Si results in restructuring [1] similar to the dewetting patterns formed when melting polymer films on Si [2]. However, in these ex-situ experiments we could only investigate the average development of the surface structure, since a new sample had to be taken for each irradiation fluence. With our new in-situ SEM/EDX at the UNILAC accelerator of GSI [3] we are now able to follow the history of individual objects from the first ion impact until their final state. The nucleation and growth mechanisms of SHI induced dewetting can now be easily studied, since the irradiation process can be controlled in very small fluence steps and dewetting stops as soon as the ion beam is switched off. This allows to immediately freeze the actual state of dewetting for careful analysis, which is hardly possible in case of liquid films. After the next irradiation step, one and the same spot can be analyzed again and such the nucleation and growth kinetics of individual dewetting holes can be determined. We will report our first results on SHI induced dewetting of iron-oxide layers with varying film thicknesses and artificial defect concentrations. [1] T. Bolse, et al., Nucl.Instr.Meth. 245 (2006), [2] S. Herminghaus, et al., Science 282

(1998), [3] S. Amirthapandian, et al., Rev.Sci.Instr. 81, (2010)

DS 42.97 Wed 15:00 P1

Model calculations for XRD at polycrystalline thin films — •Susanne Hahne, Thomas Weisemoeller, and Joachim Wollschlaeger — Department of Physics, University of Osnabrück, Barbarastr. 7, D-49069 Osnabrück, Germany

The evaluation of x-ray diffraction (XRD) data is an important method for structure determination. Regarding thin films the theoretical description of XRD is commonly based on an ideal lateral and vertical structure without defects to determine lattice constants and the film thickness. This contribution introduces a new 2D model, which includes defects of the thin film. It replaces the ideal layer with a distribution of crystallites, which cover the substrate surface completely. Their sizes are randomly distributed according to a Γ-distribution. The new model is primarily characterized by the additional dimension, which allows the reproduction of in-plane and out-of-plane data. Two types of crystallite distributions are implemented. For one type the crystallite positions are fixed to certain substrate atoms. The other type assumes a floating film. A first survey verified that the influence on the diffraction pattern of every parameter in the model is correctly reproduced. This includes a variation of the vertical lattice constant, which changes the diffraction peak position. The peaks out-of-plane are broadened, if the vertical crystallite size is decreased. For scattering vectors, which do not coincide with crystal truncation rods, strong fringes are observed. Their oscillation is strongly attenuated with a growing variance of the crystallite height distribution. Similar results are obtained with respect to the lateral crystallite sizes.

DS 42.98 Wed 15:00 P1

Surface analysis of Li-ion battery model anodes — •Andreas Seemayer, Philipp Bach, and Frank Uwe Renner — Max Planck Institut für Eisenforschung GmbH, Max-Planck-Str. 1, 40237 Düsseldorf

Lithium ion batteries are the most promising power source for future electromobility applications. Research on the battery systems aims to achieve higher rate capability, cycle life, or better safety. To achieve necessary further improvements a better understanding of the basic processes is needed. Following a surface science approach we focus on the investigation of simple model systems (like single crystals or thin film electrodes) of relevant anode materials.

We report investigations of the electrochemical insertion of Lithium in Au, Ag, Al, Mg and Si model surfaces, i.e. alloying and dealloying of Lithium alloys. As electrolyte we use the ionic liquid 1-Butyl-1-methylpyrrolidinium bis(trifluoromethanesolfonyl)imide (PYR14TFSI) with 0.3M LiTFSI. The electrochemical characterisation is performed by Cyclic Voltammetry (CV). The surface and film characterisation regarding its geometrical structure is investigated by means of Scanning Electron Microscopy (SEM) and Atomic Force Microscopy (AFM). The chemical composition is characterised ex-situ by Photoelectron Spectroscopy (PES) and Secondary Ion Mass Spectrometry (SIMS).

DS 42.99 Wed 15:00 P1

Picosecond-Pulsed Laser Deposition of $LaAlO_3$ — •Erik Thelander and Bernd Rauschenbach — Leibniz Institute of Surface Modification, Leipzig

The perovskite material $LaAlO_3$ is a dielectric with a permittivity of around 25 and a beneficial conduction band offset towards Si. Therefore it is an interesting candidate to be used as the next generation gate oxide in CMOS technology if it ever were to be grown epitaxially on Si. Here we present findings made on thin films of $LaAlO_3$, synthesized with a Pulsed Laser Deposition (PLD) process using ultrashort laser pulses, deposited both on Si and lattice matched $SrTiO_3$. Using suitable filtering techniques, we show that it is possible to avoid the incorporation of nanoparticles in the growing films which is normally a most troublesome feature of ultrashort PLD [1,2]. Film topography has been investigated with SEM and AFM, which show low particle density and smooth surfaces with RMS-values between 0.3 and 1 nm. XRD and XPS have been used to obtain structural information of the samples whereas TOF-SIMS have been employed to gain information about the diffusion in the interface as well as the elemental distribution within the films.

[1] Teghil et al., Appl. Surf. Sci., **210** (2003), 307
[2] Amoruso et al., Appl. Phys. Lett., **84** (2004), 4502

DS 42.100 Wed 15:00 P1

Contamination and Cleaning of Multilayer Mirrors with X-ray Photoelectron Spectroscopy — •Sina Gusenleitner[1,2], Marius Ernst[1,2], Dirk Ehm[2], and Friedrich Reinert[3] — [1]Universität Würzburg, Experimentelle Physik VII, D-97074 Würzburg, Germany — [2]Carl Zeiss SMT GmbH, Rudolf Eber StraSSe 2, D-73447 Oberkochen, Germany — [3]Karlsruhe Institut für Technologie (KIT), Gemeinschaftslabor für Nanoanalytik, D-76021 Karlsruhe, Germany

Extreme Ultraviolet Lithography is a promising next generation lithography technology. In this radiation regime (wavelength 13.5 nm) advanced multilayer mirrors (MLM) are used as collector and illuminator optics. The mirrors consist of a stack of alternating molybdenum and silicon layer, coated with a dedicated capping material such as Si, Ti, Mo, Pd, Ru, or their oxides. Various contamination dynamics in the lithography tool lead to formation of hydrocarbon layers on the mirror surface. In order to understand these contamination processes the adsorption, bonding and chemical environment of carbonaceous layers on MLM surfaces are investigated with X-ray Photoelectron Spectroscopy (XPS). A clean reference surface can be obtained by exposing a contaminated mirror surface to reactive species. The influence of these species on the chemical structure of the MLM surface and adsorbed carbonaceous layers was monitored with XPS. Variation of the take-off angle in XPS measurements provided information about the influence of the cleaning process on the structure of the surface, such as intermixing of the underlying layers with the capping layer material.

DS 42.101 Wed 15:00 P1

growth, characterization and bio-functionalization of cubic boron nitride thin films — •hong yin[1], lianchen shan[1], marc saitner[1], lars grieten[1], sylvia wenmackers[1], veronique vermeeren[2], fabian wilbers[1], marcel ameloot[2], luc michiels[2], marc d'olieslaeger[1,3], patrick wagner[1,3], and hans-gerd boyen[1] — [1]institute for materials research, hasselt university, wetenscharpspark 1, 3590 diepenbeek, belgium — [2]biomedical research institute, hasselt university, agoralaan buiding c, 3590 diepenbeek, belgium — [3]IMEC, division IMOMEC, wetenscharpspark 1, 3590 diepenbeek, belgium

Beside their applications as superhard coatings, in high-temperature electronics, or UV-photonics, cubic boron nitride (c-BN) thin films are also promising candidates for biological applications due to their bio-compatibility and chemical inertness. In this work, we will demonstrate that c-BN films have the potential to be used as new transducer material for biosensor applications. Impurity-free c-BN films are synthesized by means of radio frequency (r.f.) magnetron sputtering under UHV conditions. In-situ XPS and ex-situ FTIR are used as analytical tools to collect information about both, the surface and the volume parts of the films, respectively. Hydrogen-terminated films are successfully functionalized for the subsequent attachment of (amino-terminated) DNA. The successful attachment of single-stranded DNA and the subsequent hybridization to form double-stranded DNA is confirmed by supernatant fluorescence microscopy.

DS 42.102 Wed 15:00 P1

Monte Carlo Simulations for a focusing neutron guide at TOFTOF — •Roxana Valicu[1,2], Giovanna Simeoni[1,2], Peter Böni[2], Wienfried Petry[1], and Gunther Borchert[1] — [1]Forschung Reaktor München, Neutronenquelle, Lichtenbergstrasse 85747 Garching — [2]Physik-Department E21 James-Franck-Strasse 85748 Garching

TOFTOF is a direct-geometry multi-disc chopper time-of-flight spectrometer, installed at the neutron source Heinz Maier-Leibnitz FRM II. For further studies of magnetic systems and for investigation of samples under extreme conditions (high-pressure cells, electromagnetic and electrostatic levitator devices, magnetic fields) Monte Carlo simulations were performed for focusing the neutron beam and increasing the neutron flux . The gains in flux as well as the expected profile of the beam resulting from the simulations will be presented.

DS 42.103 Wed 15:00 P1

Thermal interface resistance of metal films on insulator and semi-conductor substrates measured by thermal wave techniques — •Puchong Kijamnajsuk[1], Mihai Chirtoc[2], Marc Möller[1], David Schäfer[3], Christoph Eisenmenger-Sittner[3], Detlef Spoddig[1], Ralf Meckenstock[1], and Josef Pelzl[4] — [1]Experimental Physics, University Duisburg-Essen, Germany — [2]Université de Reims Champagne-Ardenne, GRESPI-CATHERM, Reims, France — [3]Vienna University of Technology, Institute of Solid

State Physics, Wien, Austria — [4]Institute of Experimental Physics, Ruhr-University, Bochum, Germany

Thermal interfaces are essential for the application of modern composites in electronic devices. The thermal interface resistance in Cu/C and Fe/GaAs flat model systems was studied by novel approach, which relies on the frequency dependence of the photothermal signal phase and amplitude at intermediate frequencies and thermo-reflectivity. Cu-films (1 μm) were deposited by magnetron sputtering and Fe (100nm) was grown by molecular beam epitaxy. The influence of thin bonding layers (5 nm) and subsequent heat treatment on the thermal interface resistance was investigated. The bonding layer were based on B with additions of the carbide forming metals Mo, Ti and Cr. These measurements were complemented by secondary ion mass spectroscopy, scanning electron microscopy and atomic force microscopy. No correlation was found with respect to the bonding layer. A correlation was observed between adhesion strength and thermal interface resistance as well as the heat treated samples.

DS 42.104 Wed 15:00 P1

Oxidation Of Thin Metal Films For Low-cost Vacuum Quality Monitoring — •Sebastian Mäder[1], Ulrich Kunze[1], and Theodor Doll[2,3] — [1]Werkstoffe und Nanoelektronik, Ruhr-Universität Bochum, 44780 Bochum, Germany — [2]adlantis Dortmund GmbH, 44263 Dortmund, Germany — [3]Institut für Physik, Johannes Gutenberg-Universität Mainz, 55122 Mainz, Germany

Ultrathin metal films are investigated in terms of resistance changes, caused by the decrease of the electrical conductive cross section, for their application as vacuum quality sensors. Almost any pure metal is not stable in an oxygen-rich atmosphere and reacts to a metal oxide. In general, this oxide has a some orders of magnitude higher resistivity and so the growth of an oxide layer reduces the conductive path of the metal layer. For modeling the kinetics of these sensors an extended theory of metal oxidation [1,2] is used where the pressure dependence is explicitly considered. The application field of these sensors is as Vacuum Insulation Panels (VIP), which are good thermal insulators at sufficiently low inside pressure. Aluminum in the thickness range of some up to 20 nm is investigated as a metal with a compact oxide layer wherefore limiting oxide thickness and hence a long lifetime of the sensor is expected. In contrast copper is studied as a metal with a porous oxide structure, in order to yield a great resistance change in short time and therefore a better sensor response.

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[2]Boggio, J. E.; Plumb, R. C.; Surface Science **44** 3 (1966).

DS 42.105 Wed 15:00 P1

Optical switching properties and durability of a Mg-Fe alloy based thin film hydrogen sensor — •Marc K. Dietrich, Gunther Haas, André Portz, Andreas Laufer, Angelika Polity, and Bruno K. Meyer — I. Physikalisches Institut, Giessen, Germany

Mg-Fe alloy based hydrogen gas sensors were produced by a RF sputtering process. By exposure to a hydrogen containing gas mixture the Mg-metal alloy switches from the metal phase into a hydride phase, thereby the optical reflection shows a change. A Pd top layer acts as hydrogen catalyst. The degradation of the hydrogenation speed (sensor reaction) and the switching durability are well known problems of such Mg-metal based switching mirrors. Furthermore, there is a delay of sensor reaction after some weeks of storage (in air).

In order to solve these problems, we added a Ti buffer layer between MgFe and Pd layer. The buffer layer inserted sensor system featured an improvement of sensor reaction and switching durability. A polytetrafluoroethylene (PTFE) covering coat was added and reduced the sensor degeneration after the storage. Furthermore, there was an additional improvement of switching durability. Samples of PTFE/Pd/Ti/MgFe achieved over 1000 switching cycles (with 4 % hydrogen in air) without a significant performance reduction.

DS 42.106 Wed 15:00 P1

Nonvolatile bipolar resistive switching in Au/BiFeO3/Pt — •Yao Shuai[1], Shengqiang Zhou[1,2], Danilo Bürger[1], Manfred Helm[1], and Heidemarie Schmidt[1] — [1]Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, P. O. Box 510119, Dresden 01314, Germany — [2]State Key Laboratory of Nuclear Physics and Technology, School of Physics, Peking University, Beijing 100871, China

Nonvolatile bipolar resistive switching has been observed in an Au/BiFeO3/Pt structure, where a Schottky contact and an Ohmic contact were formed at the Au/BiFeO3 and BiFeO3/Pt interface, respectively. By changing the polarity of the external voltage, the Au/BiFeO3/Pt is switched between two stable resistance states with a resistance ratio larger than two orders of magnitude. Based on a systematic investigation of its electrical properties with an emphasize on its transport characteristics, a model associated with the redistribution of OVs and electron hopping process is proposed, which agrees well with our experimental observations. It is known that electron hopping usually occurs in BFO thin films and causes large leakage current, which is undesirable in traditional ferroelectric or multiferroic applications. However, it is found in the present work that the electron hopping can be controlled and utilized to realize bipolar resistive switching, which is promising for future high density memory devices.

DS 42.107 Wed 15:00 P1

The Influence of Oxygen on the Potential Distribution of Operating Zinc Oxide FETs — •Daniel Walker — TU Darmstadt, FB Materialwissenschaften, FG Elektronische Materialeigenschaften, Petersenstr 23, 64287 Darmstadt

Zinc Oxide has been studied extensively over the past 40 years and remains a material of interest for many applications including flexible electronics due to its n-type semi-conducting properties, printability from solution, transparency and wide band gap. One well known factor that has to be mitigated before commercial ZnO based electronics can be implemented is its very strong sensitivity to oxygen. This work discusses the effects of oxygen on the surface potential of an operating transistor with a highly granular ZnO film, fabricated by spin coating from solution. An ultra high vacuum Scanning Kelvin Force Microscope is used to examine at which parts of the device oxygen alters the potential distribution along the channel. It is shown that the oxygen strongly influences the behaviour of the device at the source and drain contacts and these effects are then interpreted in a qualitative model depicting the mode of operation of the transistor. The results are then related back to the conventional current-voltage characteristics.

DS 42.108 Wed 15:00 P1

Fabrication and characterization of YSZ microstructures — •Osman Khalil, Markus Piechotka, Martin Fischer, Torsten Henning, and Peter J. Klar — 1. Physikalisches Institut, Justus-Liebig-Universität, 35392 Giessen

Yttria-stabilized zirconia (YSZ) is known for its ion-conducting behaviour due to oxygen vacancies in its anion-lattice. To extract these ions from the surface a three-phase-boundary between air, YSZ and platin is desirable. Thus the conductance of an YSZ sample can be reduced by the use of thin films or by an increase of the three-phase boundary-surface. Therefore we investigated the fabrication of free-standing YSZ membranes grown on silicon by anisotropical etching of (100)-Si-wafers as well as the microstructuring of the YSZ-surface. The treatment of the samples was performed with photolithography, KOH-etching and Ar$^+$-ion-beam-etching. The samples were then investigated using AFM, SEM and optical microscopy.

DS 42.109 Wed 15:00 P1

Improvement and investigation of the emission behaviour of YSZ samples using nanostructuring and thin film technology — •Markus Piechotka, Martin Fischer, Torsten Henning, Davar Feili, and Peter J Klar — 1. Physikalisches Institut, Justus-Liebig-Universität, 35392 Giessen

We developed nano-structured free-standing YSZ-membranes for electrospray applications as well as for ion emitting purposes. YSZ is a well known solid electrolyte used widely in the production of solid oxide fuel cells (SOFC) as well as as electroceramics and possible ion emitter. Especially in the field of micro-thrust space engines, new techniques of ion emission have to be developed.

100 nm to 2 microns thin YSZ films were grown on double-side polished and thermally oxidized 2 inch silicon wafer using PLD. Subsequently photolithography structuring and wet etching with BHF and KOH were performed to lay the membrane bare. Afterwards needle structures were transferred into the YSZ-membranes using electron beam lithography followed by ion-beam etching with an Ar$^+$-beam.

The surfaces of the structured samples were investigated using AFM as well as SEM. The samples were then mounted into an integrated sample holder with multiple high voltage grids in front of the sample. This assembly functions as a solid state ion emitter with a heater as well as an oxygen supply beneath the sample. Furthermore we emitted oxygen ions from the YSZ-surface and measured the temperature dependence of the emission current as well as the ion energy distribution with Faraday cups and with a retarding potential analyser.

DS 42.110 Wed 15:00 P1

Zelladhäsive Plasmapolymerschichten aus Ethylendiamin — •Holger Testrich, Steffi Kaledat, Mario Dünnbier und Jürgen Meichsner — Universität Greifswald, Institut für Physik, Felix-Hausdorff-Str. 6, D-17487 Greifswald

Dünne Plasmapolymerschichten mit einer Schichtdicke zwischen 50 und 100 nm wurden in einer asymmetrischen, kapazitiv gekoppelten Hochfrequenzentladung in einem Gemisch aus Argon und Ethylendiamin (EDA) hergestellt. Die plasmachemischen Stoffwandlungsprozesse wurden mit der optischen Emissionsspektroskopie, FTIR Spektroskopie und Massenspektrometrie untersucht. Die Charakterisierung der Schichteigenschaften erfolgte mittels Ellipsometrie, IRRAS und XPS. Die optische Emission des Plasmas ist neben charakteristischen Ar-Linien durch eine zunehmende Intensität von CN-Banden bestimmt. Stabile gasförmige Reaktionsprodukte sind insbesondere NH3, HCN und H2. Die dünnen plasmapolymerisierten Schichten aus EDA besitzen einen hohen Stickstoffanteil (N/C ca. 40%) und zeigen charakteristische IR-Absorptionsbanden der N-H, C-H und C-N Molekülschwingungen. Eine Lagerung an Luft führte zu einer Alterung der Schichten, wobei insbesondere sauerstoffhaltige Gruppen nachgewiesen wurden. Die Beschichtung von biomedizinisch relevanten Substraten (Implantate) führte zu einer signifikanten Erhöhung der Adhäsion und Ausbreitung von humanen Knochenzellen. Gefördert im Campus PlasmaMed, Nr.13N9774.

DS 42.111 Wed 15:00 P1

Attosecond pulse-shaping including control of the attochirp by aperiodic extreme ultraviolet multilayer mirrors — •Michael Hofstetter[1,2], Alexander Guggenmos[1,2], Eleftherios Goulielmakis[1], Martin Schultze[1,2], Elisabeth Magerl[1], Stefan Neppl[3], Elisabeth Bothschafter[1,3], Markus Fiess[1], Benjamin Dennhardt[3], Justin Gagnon[1,2], Vladislav Yakovlev[1,2], Reinhard Kienberger[1,3], Adrian Cavalieri[1], Ralph Ernstorfer[1,3], Ferenc Krausz[1,2], and Ulf Kleineberg[1,2] — [1]MPQ, Garching, Germany — [2]LMU, Garching, Germany — [3]TUM, Garching, Germany

Attosecond physics allow to reveal the dynamics of elementary electronic processes with never before enterable precision. Multilayer XUV mirrors are the key components to shape all attosecond pulse parameters as its central energy, spectral bandwidth, pulse length and attochirp with a high degree of freedom. This allows us to investigate and compare resonant and non-resonant electronic transitions in solids, surfaces, molecules and gases, as each experiment requires its perfectly synchronized pulse and test current physical models. We will present our latest results on shaping attosecond pulses in the spectral range between 80 and 140 eV from gas high harmonics, characterized via FROG analyses of electron streaking. We will present explicit examples of dispersion control using chirped XUV multilayers. We will further present ideas on attosecond spectral cleaning that enable experiments with high temporal (few 100 as) and high spectral (few eV) resolution and clearly reduced noise.

DS 42.112 Wed 15:00 P1

Simulation of the ultrafast nonlinear optical response of metal slabs — •Mathias Wand, Torsten Meier, and Jens Förstner — Department Physik and CeOPP, Universität Paderborn, 33098 Paderborn, Germany

With the current rise of interest in plasmonic nanostructures [1], it has become apparent that the nonlocal and nonlinear optical properties of such systems can only be described properly by theoretical models beyond the classical free-electron Drude model.

We present a nonequilibrium ab initio method for calculating nonlinear and nonlocal optical effects in metallic slabs with a thickness of several nanometers. The numerical analysis is based on the full solution of the time-dependent Kohn-Sham equations [2] for a jellium system and allows to study the optical response of metal electrons subject to arbitrarily shaped intense light pulses. We find a strong localization of the generated second-harmonic current in the surface regions of the slabs [3].

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2. A. Castro, M.A.L. Marques, and A. Rubio, J. Chem. Phys. 121, 8 (2004).
3. M. Wand, A. Schindlmayr, T. Meier, and J. Förstner, phys. stat. sol., submitted (2010).

DS 42.113 Wed 15:00 P1

A study on nanocomposites made of a conducting polymer and metallic nanoparticles — •rania mohammed ahmed khalil[1,2], ramzy abdelaziz mahmoud abdelaziz[1], thomas strunkus[2], franz faupel[2], and mady elbahri[1,3] — [1]Nanochemistry and Nanoengineering, Institute for materials science, Faculty of engineering, Christian-Albrechts-University of Kiel — [2]Multicomponent materials, Institute for materials science, Faculty of engineering, Christian-Albrechts-University of Kiel — [3]Helmholtz-Zentrum Geesthacht GmbH, Institute of Polymer Research, Nanochemistry and Nanoengineering

Conducting polymers offer a unique combination of properties that makes them attractive materials for many electronic applications. PEDOT:PSS is one of the most successful conductive materials which is considered to be highly stable and resisting degradation under typical ambient conditions. In this study, we have prepared two sets of conducting polymer nano-composites. The first set is composed of PEDOT:PSS doped with different aspect ratios of gold nanorod and the other one is PEDOT:PSS doped with different sizes of gold nanosphere. The chemical reduction method was used for preparing the nano-particles. Indeed, gold nanorods and nanosphere which exhibit tunable absorption as a function of their size and aspect ratio, respectively, have tuned the absorption coefficient for PEDOT: PSS. The nature of the dopant as well as the degree of doping has played a significant role in the improvement of the electrical conductivity of conducting polymer.

DS 42.114 Wed 15:00 P1

Mueller matrix ellipsometry on large area split ring resonator arrays — •Bruno Gompf, Barbara Krausz, Bettina Frank, Harald Giessen, and Martin Dressel — Physikalisches Institut and Research Center SCOPE, Universität Stuttgart

The workhorse of the metamaterial community is the split ring resonator (SRR). It represents the top-down approach to tailored effective optical parameters in the sense that it is essentially a miniature inductive-capacitive resonant circuit. Arranging many of these nanocircuits, sometimes called photonic atoms, together, it is assumed that they merge into a material with effective optical parameters. The problem is that in general the optical response is k-dependent, only in the special case when the regular building blocks of a material (molecules, unit cells, nanostructures, etc.) are small compared to the wavelength, spatial dispersion can be neglected. Surprisingly the complete k-dependent optical response of SRR-arrays was not measured up to now. We present Mueller matrix spectroscopic ellipsometry on large area SRR arrays in transmission at various angles of incidence and azimuthal orientations in the energy range of 0.73 to 4.6eV. To visualize the experimental results, we plot the matrix elements in polar coordinates. From the off-diagonal elements, it becomes obvious that the SRR-array is birefringent, but with strongly k-dependent optical axes. Closed ring structures, fabricated in the same way, do not exhibit this behaviour. The results clearly show that the optical response of the SRR array cannot be described by purely dielectric effective parameters.

DS 42.115 Wed 15:00 P1

Theory of the Spatiotemporal Control of Optical Excitations in Metal Nanostructures — •Felix Schlosser[1], Mario Schoth[1], Sven Burger[2], Frank Schmidt[2], Andreas Knorr[1], Shaul Mukamel[3], and Marten Richter[1,3] — [1]Institut für Theoretische Physik, Technische Universität Berlin, Germany — [2]Zuse-Institut Berlin, Germany — [3]Department of Chemistry, University of California, Irvine, USA

Spatiotemporal control of electronic excitations with subwavelength precision is a useful technique in modern experiments. It can be achieved by combination of pulse shaping techniques for ultrashort laser pulses with nanoplasmonics [1]. In order to describe the linear and nonlinear excitation and response of metal nanostructures on a fundamental level, a microscopic material model is combined with a Maxwell solver (JCMwave, Zuse-Institut Berlin) to simulate the spatiotemporal control caused by shaped pulses [2] including phase control optimized by a genetic algorithm. As a first application, we demonstrate that the precise control of excitations in coupled semiconductor quantum dots opens new possibilities for coherent spectroscopy: In particular, we discuss a double quantum coherence (DQC) method [3] enhanced by the additional spatial control, which will reveal more information about the delocalized excitonic wave functions in coupled nanostructures compared to DQC without spatial control.

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[2] M. Reichelt and T. Meier, Opt. Lett. **34**, 2900-2902 (2009)
[3] L. Yang and S. Mukamel, Phys. Rev. Lett. **100**, 057402 (2008)

DS 42.116 Wed 15:00 P1

Silver on nanostructured quartz as reusable SERS-active substrates — •Henrik Schneidewind[1], Karina Weber[2], Matthias Zeisberger[1], Uwe Huebner[1], Dana Cialla[2], Roland Mattheis[1], and Juergen Popp[1,2] — [1]Institute of Photonic Technology Jena (IPHT), Albert-Einstein-Strasse 9, 07745 Jena, Germany — [2]Institute of Physical Chemistry, Friedrich-Schiller-University Jena, Helmholtzweg 4, 07743 Jena, Germany

We investigated reusable substrates for Surface Enhanced Raman Spectroscopy (SERS) comprising of nanostructured gratings in quartz coated with silver films. The contribution involves the ED modelling of suited structures, there preparation, and some exemplary SERS results. Although the shown structures were prepared by means of electron lithography they offer the opportunity for easy and economical fabrication using e.g. imprint techniques. We show the influence of technological parameters as well as of thin film properties on the SERS enhancement of the structures. A homogeneous enhancement exceeding 10^5 is possible across large areas. The SERS enhancement is clearly caused by surface plasmons generated in consequence of the periodic structures and not by surface roughness.

DS 42.117 Wed 15:00 P1

Femtosecond pump-probe spectroscopy of the dielectric function of a polymer matrix with embedded gold nanoparticles — •Mareike Kiel[1], Steffen Mitzscherling[1], and Matias Bargheer[1,2] — [1]Institut für Physik, Universität Potsdam, Germany — [2]Helmholtz Zentrum Berlin, Germany

We investigate a well characterized multilayered compound system [1] of polyelectrolytes and gold nanoparticles with femtosecond pump-probe spectroscopy. The transient absorption A(t) and reflection R(t) after heating the electrons with an intense femtosecond laser pulse are measured simultaneously. We test the well known theoretical model that ascribes the observed signals to the smearing of the Fermi-edge of the conduction electrons by a quantitative comparison to the simultaneously measured A(t) and R(t). In a separate evaluation scheme we directly derive the real and imaginary part of the dielectric function of the composite material from the experiment. A detailed comparison of the two approaches is given.

[1] M. Kiel et al., Langmuir 26, 18499 (2010)

DS 42.118 Wed 15:00 P1

Plasmon-Polariton modes of dense Au nanowire arrays — •Hongdan Yan[1], Peter Lemmens[1], Dirk Wulferding[1], Mehmet Fatih Cetin[1], Sabine Tornow[2], Gertrud Zwicknagl[2], Ulrich Krieg[3], Herbert Pfnür[3], Winfried Daum[4], Gerhard Lilienkamp[4], and Meinhard Schilling[5] — [1]IPKM, TU-BS, Braunschweig, Germany — [2]IMP, TU-BS, Braunschweig, Germany — [3]IFP, LU Hannover, Germany — [4]IEPT, TU Clausthal, Germany — [5]EMG, TU-BS, Braunschweig, Germany

Using optical absorption and other techniques we study plasmon-polariton modes of dense Au nanowire arrays as function of geometrical parameters and coupling to molecular degrees of freedom. For this instance we electrochemically deposit Au nanowires in porous alumina with well controlled morphology and defect concentration. Transverse and longitudinal modes are observed in the absorption spectra resulting from the anisotropic plasmonic structure. The longitudinal mode shows a blue shift of energy with increasing length of the wires due to the more collective nature of this response. We compare our observations with model calculations and corresponding results on 2D Ag nanowire lattices.

Work supported by IGSM and NTH.

DS 42.119 Wed 15:00 P1

Simulation of Plasmonic Microcavities — •Sven Burger, Lin Zschiedrich, Jan Pomplun, and Frank Schmidt — Zuse Institute Berlin, Berlin, Germany

Plasmon-based waveguiding structures allow for transport and storage of light at subwavelength scales. Fast and accurate 3D Maxwell solvers are needed for designing structural parameters of, e.g., hybrid plasmonic waveguides. Due to the multi-scale nature of the corresponding field distributions, accurate computation of the properties of such devices can be numerically challenging.

We have developed finite-element method (FEM) based solvers for the Maxwell eigenvalue and scattering problems. The method is based on higher order vectorial elements, adaptive unstructured grids, and on a rigorous treatment of transparent boundaries. The method has been applied to plasmonic devices like plasmonic antennas, gratings and waveguides [1-5]. Here we present 3D simulations of light propagation in plasmonic waveguides and plasmon laser cavities. We investigate the accuracy of the simulations in a convergence analysis of the numerical results.

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DS 42.120 Wed 15:00 P1

Fabrication of diffractive XUV optics and plasmonic nanostructures by e-beam lithography — •Christian Späth[1], David Kronmüller[1], Jürgen Schmidt[1], Soo Hoon Chew[1], Michael Hofstetter[2], Alexander Guggenmos[2], Mihael Kranjec[1], and Ulf Kleineberg[1,2] — [1]Fakultät für Physik, Ludwig-Maximilians-Universität München, 85748 Garching, Germany — [2]Max-Planck-Institut für Quantenoptik, 85748 Garching, Germany

E-beam lithography is one of the premier choices for fabricating artificial structures on the nanometer scale and is widely used in the field of electronics and nanophotonics. We are reporting about our latest results in the development of diffractive nanostructures for sub-μm focusing of coherent XUV high harmonic radiation at around 95 eV photon energy. Zone Plate patterns (D=120 μm, N = 120) have been written in PMMA and HSQ resist on Si(100) wafer and have subsequently been coated with a Mo/Si multilayer resulting in a reflective nanofocusing device. These structures have been characterized by means of atomic force and scanning electron microscopy. Furthermore bow-tie nanostructures for local near field enhancement of ultrashort femtosecond laser pulses have been fabricated in PMMA and were transferred in 30 nm Ag by Lift-Off. These silver nanostructures were investigated by AFM as well as 1P-PEEM and 2P-PEEM.

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Electrical and structural properties of SrTiO3 / Sr-based conducting films on microwave suitable carriers — •Kyrylo Greben[1], Eugen Hollmann[1], Thomas Grellmann[1], Rolf Kutzner[1], Oleksandr Prokopenko[2], Vladimir Pan[3], and Roger Wördenweber[1] — [1]Institute of Bio- and Nanosystems (IBN), Forschungszentrum Jülich, D-52425 Jülich, Germany — [2]Radiophysics Faculty of Taras Shevchenko National University of Kyiv, 2, Acad. Glushkov Ave., building 5, 03127, Kyiv, Ukraine — [3]Institute for Metal Physics, National Academy of Sciences of Ukraine, 36 Vernadsky Street, Kiev, 03142, Ukraine

The aim of this work is the preparation of microwave suitable thin film devices consisting of a conducting base layer covered by a high-k oxide layer. Different systems are considered. Here we mainly report on the system consisting of r-cut sapphire or LaAlO3, SrRuO3 or Nb:SrTiO3, and SrTiO3 as a substrate, conductor, and high-k layer, respectively. In order to achieve epitaxial growth, the sapphire is covered with a (002) CeO2 buffer layer. Bottom electrodes and high-k SrTiO3 are deposited via rf magnetron sputter technique. Depending on the choice of parameters various phases and structural orientations are obtained for the base layer resulting in a large variation in the specific resistance. Finally, SrTiO3 layers are deposited onto the bottom electrodes layers. The resulting structural and electronic properties of both layers are determined via RBS, XRD analysis and cryoelectronic analysis, respectively.

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Dielectric function of ultra-thin high-k films grown by atomic layer deposition — •Li Ding[1], Lin Chen[2], Marion Friedrich[1], Ovidiu Gordan[1], Wei Zhang[2], and Dietrich Zahn[1] — [1]Semiconductor Physics, Chemnitz University of Technology, D-09107, Germany — [2]State Key Laboratory of ASIC and System, Department of Microelectronics, Fudan University, Shanghai 200433, China

High-k dielectrics are intensively studied to replace the conventionally used SiO2 as gate dielectrics in various electronic devices [1]. Hafnium dioxide (HfO2) is one of the candidates due to a high k value, a wide band gap around 6.4 eV, and a good thermal stability [2]. HfO2 usually forms crystalline structures, but amorphous films are preferred to minimize leakage currents through dielectric layers. It is possible to obtain amorphous films by growing HfO2 together with another compound, such as Al2O3, which stays amorphous at much higher temperatures.

Two series of samples were prepared by atomic layer deposition (ALD). One series consists of alloy films with different component ratios between HfO2 and Al2O3, while the other consists of bilayer films with various layer thicknesses. In order to investigate the influence of the film thickness and layer structure on the band gap, a vacuum ultraviolet (VUV) ellipsometer (4.0-9.8 eV) is employed using synchrotron radiation as a light source. Moreover, a laboratory spectroscopic ellipsometer (0.7-5 eV) is used to determine the film thickness.

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Admittance spectroscopy to characterize interface traps in MOS structures containing high-k materials — •Markus Hippler[1], Jan Lehmann[1], Varun John[1], Wolfgang Skorupa[1], Manfred Helm[1], Heidemarie Schmidt[1], Marcelo Lopes[2], Jürgen Schubert[2], and Siegfried Mantl[2] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Bautzner Landstraße 400, 01314 Dresden — [2]PGI-9 and JARAFIT, Research Centre Jülich, 52425 Jülich

Today‘s planar metal-oxide-semiconductor field-effect transistor (MOSFET) technology with silicon dioxide (SiO2) as the gate dielectric has reached its limit of scaling, because the leakage currents through 1nm SiO2 are unacceptable. For an ongoing down-scaling process, the gate dielectric has to be exchanged by a material with a higher relative dielectric constant k. Two of those candidates are lanthanum lutetium oxide (LLO) and lanthanum scandate oxide (LSO) with relative dielectric constants of k(LSO)=24 and k(LLO)=32, respectively. Here we characterize the properties of the interface traps, i.e. the trap density and time constant of MOS diodes based on those materials by admittance spectroscopy. For this purpose 6 and 20nm thick layers of LLO and LSO layers have been grown by molecular beam deposition (MBD) on RCA-cleaned p-Si.The admittance measurements were performed in the frequency range from 50 Hz to 20 kHz with an AC test bias amplitude of 10mV under variation of the DC ground voltage. Measured data have been analyzed by a numerical fitting program with respect to the serial resistance Rs and oxide capacitance Cox.

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Ab initio study of the silylation mechanism of OH-groups with different Silazanes — •Oliver Böhm[1,2], Roman Leitsmann[1], Philipp Plänitz[1], Christian Radehaus[1], Michael Schreiber[2], and Matthias Schaller[3] — [1]GWT-TUD GmbH, Material Calculations, Chemnitz, Germany — [2]Institut für Physik, Technische Universität Chemnitz, 09107 Chemnitz — [3]Globalfoundries Dresden Module Two GmbH & Co. KG, Germany

The decreasing feature size of integrated circuits results in a smaller distance between the conduction layers, which is accompanied by an increasing resistance capacitance delay. Therefore, the usage of materials with an ultra low dielectric constant is necessary. However, the application of such ultra low k (ULK) materials is connected to several problems, like the formation of OH-groups after the etch process. This results in moisture uptake and a strongly increasing dielectric constant. To restore the k-value, a post-etch treatment is necessary. In this study we investigate the silylation of OH-groups with different silazanes. In particular we use density functional theory to study the different reaction mechanisms. For the silylation reaction of Hexamethyldisilazane (HMDS) and Trimethylaminosilane (TMAS) with Silanol, the minimum energy paths as well as the transition states are discussed in detail.

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Thermal stability of BaSrO thin films and the influence of Al intermediate layers to the electrical properties of high-k Si(001)/BaSrO/Au MOS diodes — •Shariful Islam[1], Dirk Müller-Sajak[1], Alexandr Cosceev[2], Herbert Pfnür[1], and Karl R. Hofmann[2] — [1]Leibniz-Universität Hannover, Inst. f. Festkörperphysik — [2]Leibniz-Universität Hannover, Bauelemente der Mikro- und Nanoelektronik

MOS diodes with crystalline $\mathrm{Ba_{0.7}Sr_{0.3}O}$ gate oxide and Au gate metal on n- and p-Si(001) were produced, which have a dielectric constant of $\epsilon_r \approx 28$. The oxides were grown on structured Si(001) in a UHV chamber by MBE in oxygen ambient conditions and capped with 100nm Au for ex-situ electrical measurements. I-V measurements show low leakage currents compared to $\mathrm{SiO_2}$ with the same EOT. From C-V measurements we extracted with the Terman method a density of interface states, D_{it}, of only $\approx 10^{10}\mathrm{eV}^{-1}\mathrm{cm}^{-2}$.

We tested the thermal stability of these oxides and investigated them with X-Ray Photoelectron Spectroscopy (XPS). They are fully stable up to 450°C but convert to other chemical species, most likely silicates, at higher temperatures. But even at 700°C no formation of $\mathrm{SiO_2}$ at the interface to Si was detectable.

To improve the adhesion between the Au gate metal and the oxide we evaporated a thin layer of Al at the Au/oxide interface. This causes a thickness dependent shift of the flatband voltage. We will present our XPS measurements of the chemical origin of this shift.