DS 29: Poster: Molecular Spintronics, Biomolecular and Functional Organic Layers, Organic Electronics and Photovoltaics, Plasmonics and Nanophotonics, Organic Thin Films, Nanoengineered Thin Films, Thin Film Characterisation,

Time: Wednesday 15:00–17:30 Location: Poster A

DS 29.1 Wed 15:00 Poster A

In-situ monitoring the growth of sexithiophenyl on Ag(110) by fast reflectance difference spectroscopy — Chunguang Hu[1,2], •Lidong Sun[1], Michael Hohage[1], and Peter Zeppenfeld[1] — [1]Institut für Experimentalphysik, Johannes-Kepler-Universität Linz, Austria — [2]State Key Lab of Precision Measuring Technology and Instruments, Tianjin University, China

A rotating compensator based reflectance difference spectrometer (RCRDS) has been developed for fast spectroscopic measurement of the evolution of optical properties of surfaces and thin films. As an example, the application of this new spectrometer to the in-situ monitoring the growth of sexithiophenyl (6T) thin films on Ag(110) will be reported. The evolution of the optical properties, i.e., absorption and polarization, of 6T thin films during growth are measured with a time resolution of 10 seconds in the photon energy range between 1.5 and 4.5 eV. The RD spectra show clearly that 6T grows on Ag(110) in a Stranski-Krastanov mode with a 2 ML thick wetting layer. Specifically, 6T molecules are lying flat on the surface and the long molecular axis in condensed phase is orientated preferentially along the [001] direction of Ag(110). The results demonstrate that RCRDS is a versatile tool for the in-situ, real time studies of thin film growth revealing detailed information on the nucleation and growth, as well as the molecular orientation and interactions.

DS 29.2 Wed 15:00 Poster A

Photoluminescence in coevaporated pentacene- perfluoropentacene films — •Falk Anger[1,2], J. Oriol Ossó[2], Ute Heinemeyer[1], Katharina Broch[1], Abel Roigé[2], Reinhard Scholz[3], Alexander Gerlach[1], and Frank Schreiber[1] — [1]Institut für Angewandte Physik, Auf der Morgenstelle 10, 72076 Tübingen — [2]MATGAS 2000 AIE, Campus de la UAB, 08193 Bellaterra — [3]Walter Schottky Institut, Technische Universität München, Am Coulombwall 3, 85748 Garching

One of the crucial issues in complex organic electronic device structures is that of the coupling between different organic components. This is not only relevant for device applications, but also important from a fundamental point of view, since many properties, whether charge transport or optical spectra depend on the molecule-molecule coupling.

We present a study of the intermolecular coupling in films of pentacene (PEN) and perfluoropentacene (PFP) single and coevaporated films, which form organic donator-acceptor systems. The structural similarity of PEN and PFP is expected to promote intermixing and thus the chance of spectral coupling. The photoluminescence spectra of the coevaporated films on SiO_2 and ITO reveal pronounced optical coupling effects which depend on the mixing ratio of the molecules. New features appear in the spectra, which cannot be explained by using a linear combination of the spectra of the individual components. These coupling effects and ideas for their interpretation are discussed based on spectra at high and low temperature under vacuum atmosphere.

DS 29.3 Wed 15:00 Poster A

Spectroelectrochemical Characterization of Thin Films of Hexadecafluorophthalocyaninatozinc Prepared by Vapour Deposition — •Mareike Falk, Stefanie Nagel, Christopher Keil, and Derck Schlettwein — Institute of Applied Physics, Justus-Liebig-University Giessen, Germany. email:schlettwein@uni-giessen.de

Thin films (10-100nm) of hexadecafluorophthalocyaninatozinc(II) ($F_{16}PcZn$) were prepared by vapour deposition. The films were characterized by cyclic voltammetry in 1M $LiCl$ as electrolyte with concomitant UV/Vis spectroscopy. Potential was applied between 0.6 and -1.1 V vs. SCE and scan rate was varied from 2 to 100 mV/s. During reduction of $F_{16}PcZn$ in a first step a radical anion was formed and in a second step a dianion was generated. For charge balance Li^+ counter ions were intercalated into the film. During the first cycles in cyclic voltammetry of freshly prepared films the initiation of the films could be monitored by the increase of the charge uptake most likely caused by the successive expansion of the structure due to intercalation of lithium ions as charge balancing ions. After the initiation the films remained stable and a nearly reversible reaction could be observed. The current densities of the reduction and reoxidation peaks showed linear dependence on the square root of scan rate which indicated the diffusion of counter ions in the films as the rate determining step.

DS 29.4 Wed 15:00 Poster A

Model supported generation of Reflection Anisotropy Spectra of copper phthalocyanine films on isotropic and anisotropic silicon substrates — •Falko Seidel, Li Ding, and Dietrich R. T. Zahn — Semiconductor Physics, Chemnitz University of Technology, D-09107 Chemnitz, Germany

Reflection Anisotropy Spectroscopy (RAS) and Spectroscopic Ellipsometry (SE) are two techniques which measure the change in polarization after reflection of light at a sample surface. The main difference between them is the fact that in RAS an incidence angle near 0° is used while in SE the angle of incidence is usually in range close to the Brewster angle. Eventually the real and imaginary part of the RA spectra can be transformed into the well known Ψ and Δ values obtained from SE. Hence, the evaluation procedure of RA spectra can be performed in a similar way as for SE. Since interference enhances the RA signal of thin films, the measurements can lead to incorrect interpretation of features when interference comes into play. For this reason in this work a simulation of anisotropic copper phthalocyanine films on flat Si(111), vicinal Si(111) with 6° off-cut angle, and on a Si(110) substrate is performed. The main aim is to get an idea about the origin of the RAS features if the substrate is also anisotropic. The results allow real anisotropy features and interference induced ones to be distinguished.

DS 29.5 Wed 15:00 Poster A

Influence of electric and magnetic fields during film growth of phthalocyanines — •Florian Latteyer[1], Vladimir Plyashkevich[2], Tamara Basova[2], Heiko Peisert[1], and Thomas Chassé[1] — [1]University of Tübingen, Institute for Physical and Theoretical Chemistry, Tübingen, Germany — [2]Nikolaev Institute of Inorganic Chemistry, Novosibirsk, Russia

Due to their remarkable physical and chemical properties, phthalocyanines (Pcs) are discussed for applications in devices such as organic solar cells, organic field effect transistors, organic light emitting diodes etc. because of their easy substitutions with side chains to tailor their properties. Many planar, non-substituted Pcs have a molecular point group of D4h, there are several representatives of this class of molecules which are non-planar and exhibit C4v symmetry resulting in a permanent electric dipole moment. As a consequence, the presence of electric fields can affect growth of these molecules[1]. Since Pcs posses a high delocalized conjugated pi-system, a ring current could be induced into this pi-system by applying exterior magnetic fields[2].

Thin films of different planar and non-planar Pcs are prepared in UHV applying electric and magnetic fields during organic molecular beam deposition. The molecular orientation in these films was studied by polarized Raman- and optical spectroscopy as well as AFM.

[1]Schuster, B. E.; Basova, T. V.; Peisert, H.; Chassé, T. Chemphyschem 2009, 10, 1874.

[2]Kolotovska, V.; Friedrich, M.; Zahn, D. R. T.; Salvan, G. J. Cryst. Growth 2006, 291, 166.

DS 29.6 Wed 15:00 Poster A

In-situ Optical Spectroscopy During the Growth of Phthalocyanine Thin Films on Single Crystalline Substrates — •Enno Lorenz[1], André Dragässer[1], Christopher Keil[1], Jens Wallys[2], Martin Eickhoff[2], and Derck Schlettwein[1] — [1]Institute of Applied Physics, Justus-Liebig-University Giessen, Germany. email:schlettwein@uni-giessen.de — [2]Experimental Physics I, Justus-Liebig-University Giessen, Germany.

Thin films of differently substituted metal phthalocyanines were grown on alkali halide (NaCl, KCl and KBr) 001 faces and on wurtzite GaN 0001 on sapphire by physical vapor deposition. The films were studied during growth from the monolayer thickness regime to an average film thickness of 100 nm. Since phthalocyanines are characterized by a large oscillator strength of the electronic transition following absorption of visible light and by strong intermolecular dipole coupling of the transition dipoles in the solid state, optical measurements are well suited to study the development of intermolecular coupling and crystal structure during film growth. In- situ optical analysis was performed in transmission geometry perpendicular to the molecular deposition beam to achieve sub- monolayer sensitivity. The results are discussed in context of structural and morphological characteristics of the observed films.

DS 29.7 Wed 15:00 Poster A

Structure optimization of pentacene thin film transistors controlled by substrate temperature and annealing — •Tossapol Tippo[1], Chanchana Thanachayanont[2], Steffen Schulze[3], Michael Hietschold[3], and Apinunt Thanachayanont[1] — [1]Faculty of Engineering and College of Data Storage Technology and Applications, King Mongkut's Institute of Technology Ladkrabang, Chalongkrung Road, Ladkrabang Bangkok 10520, Thailand — [2]National Metal and Materials Technology Center, Thailand Science Park, Klong 1, Klong Luang, Pathumthani 12120, Thailand — [3]Chemnitz University of Technology, Solid Surface Analysis Group, D-09107 Chemnitz, Germany

Pentacene thin film transistors (TFTs) were fabricated by thermal evaporation of the organic molecules. The structure of the vacuum deposited pentacene thin films is very sensitive to numerous deposition parameters. The pentacene thin films were characterized to study the effect of substrate temperature during the deposition in order to maximize grain sizes and the effect of annealing to improve the current paths through the grains of pentacene thin films. Scanning electron microscopy indicated that the higher substrate temperature resulted in the larger grain size. Subsequent annealing enhances dense packing of grains by reducing the space between them. The results also suggested that the evolution of the film growth is very sensitive to the crystal quality of the initial state of growth close to the substrate film interface.

DS 29.8 Wed 15:00 Poster A

Trap-state influence on charge carrier transport in perylene based OTFTs — •Christian Effertz, Ingolf Segger, Philip Schulz, and Matthias Wuttig — Institute of Physics (IA), RWTH Aachen University of Technology, 52056 Aachen, Germany

Organic Thin-Film Transistors (OTFTs) have been intensively researched due to their adaptability, e.g. as an active matrix for flexible displays or in low-cost RFID (Radio-Frequence-Identification) tags. Recent reports indicate that OTFTs can match their inorganic counterparts based on hydrogenated amorphous silicon (a-Si:H) in terms of mobility and I_{on}/I_{off}-ratio.

In order to gain a deeper insight in the yet not fully understood charge carrier transport in organic thin-film devices, we have produced and investigated perylene based bottom-gate top-contact OTFTs. Our measurements, including temperature dependent transfer characteristics, time-domain- and temperature-stimulated current, show a profound influence of trap-states on charge transport in organic electronic devices. For a more detailed study of the influence of trap-states on transistor characteristics, model calculations were carried out.

DS 29.9 Wed 15:00 Poster A

Tailoring ferroelectric interfaces: surface modification of PZT mediated through functionalized thiophene derivates — •Peter Milde[1], Kinga Haubner[2,3], Evelyn Jähne[3], Denny Köhler[1], Ulrich Zerweck[1], and Lukas M. Eng[1] — [1]Department of Applied Photophysics, TU Dresden, Dresden, Germany — [2]Leibniz Institute for Solid State and Materials Research Dresden, TU Dresden, Dresden, Germany — [3]Institute of Macromolecular Chemistry and Textile Chemistry, TU Dresden, Dresden, Germany

Organic field effect transistors (OFETs) with a gate "electrode" that is made out of a ferroelectric (FE) have become a field of intense research [1]. Non-volatile memory functionality is expected due to the strong and remanent electric field arising from bound surface charges at the FE/molecular interface. In order to achieve excellent electric transport properties, a high degree of intermolecular ordering is inevitable. In our approach, lead zirconate titanate (PZT) is used as material of choice for the design of an ultra-thin ferroelectric gate electrode in a Ferroelectric-OFET. The focus of the present work lays on the growth process of the molecularly thin organic conduction layer, based on α,ω-dicyano-β,β*-dibutylquaterthiophene (DCNDBQT). Film formation is effectively promoted through specifically designed, bifunctional self-assembling molecules (CNBTPA: 5-cyano-2-(butyl-4-phosphonic acid)-3-butylthiophene) which act as template layer. We report on nc-AFM and KPFM investigation of the template layer's structural and electronic properties.

[1] R. Tamura et al., Thin Solid Films 516, 2753 (2008)

DS 29.10 Wed 15:00 Poster A

Characterization of various Oligothiophenes for their suitability in organic field-effect transistors (OFETs) — •Vera Hoffmann[1], Peter Milde[1], Kinga Haubner[2], Evelyn Jaehne[3], Ulrich Zerweck[1], and Lukas M. Eng[1] — [1]Department of Applied Photophysics, TU Dresden, Dresden, Germany — [2]Leibniz Institute for Solid State and Material Research Dresden, TU Dresden, Dresden, Germany — [3]Institute of Macromolecular Chemistry and Textile Chemistry, TU Dresden, Dresden, Germany

Self-assembled molecular monolayers are inevitable for nano-scaled organic electronic devices [1, 2]. Non-contact atomic force microscopy (nc-AFM) in combination with Kelvin-probe force microscopy (KPFM) yields access to information about structural and electronic properties of such self-assembled monolayers [3].

In the present study, we investigate thiophene derivatives for their perspective use in organic field-effect transistors. Dihexylsexithiophene (DHST) monolayers are prepared by physical vapour deposition on TiO_2 and SiO_2 substrates having source/drain gold electrode structures. In situ high resolution KPFM and topography measurements of operating OFET devices are shown and discussed with respect to their future suitability.

[1] Smits et al., nature 455, 956 (2008)
[2] Haubner et al., phys. stat. solidi A 205, 430 (2008)
[3] Zerweck et al., Phys. Rev. B 71, 125424 (2005)

DS 29.11 Wed 15:00 Poster A

Growth and Structure of tetrazine based organic thin films — •Dominik Meyer[1], Philip Schulz[1], Martin Reininghaus[1], Pierre Audebert[2], and Matthias Wuttig[1] — [1]Institute of Physics (IA), RWTH Aachen University of Technology, 52056 Aachen, Germany — [2]PPSM (CNRS UMR 8531), Ecole Normale Supérieure de Cachan, 61, avenue de Président Wilson, 94235 Cachan Cedex, France

In semiconductor and sensor technology, a variety of organic molecules have been explored for optoelectronic applications such as organic LEDs or TFTs. Tetrazines are aromatic molecules, which are comprised of a benzene ring where four carbon atoms are replaced by nitrogen, leading to an electron–poor delocalized electronic system that provides a high electron affinity. This structure may provide very interesting properties, i. e. luminescence and reversible electroactivity, thus rendering these molecules promising for use in sensor applications [1].

In this study we investigate the structural properties of tetrazine thin films, evaporated under high vacuum conditions on Au(111) substrates. X-ray Diffraction and Fourier transformed infrared spectroscopy been employed to explore the growth of the deposited organic layer. In order to describe the recorded IR spectra and conclude on the molecular orientation density functional theory calculations were performed. By tuning deposition parameters and surface conditions of the underlying substrate, we were able to realize different growth scenarios and tailor the film perfection with respect to the structural ordering.

[1] Kim, Y.; Kim, E.; Clavier, G.; Audebert, P. Chem. Commun., 2006, 3612–3614

DS 29.12 Wed 15:00 Poster A

Template induced-ordering of perfluoropentacene films — •Tobias Breuer and Gregor Witte — Molekulare Festkörperphysik, Philipps-Universität Marburg, 35032 Marburg, Germany

Perfluorination of pentacene offers a promising route to produce an n-type organic semiconductor with promising electronic properties which further has the advantage of being stable against oxidation thus making this material interesting for device applications [1]. On SiO2 substrates perfluoropentacene (PFP) forms needle-like islands with (100) texture which are azimuthally isotropic oriented [2]. In order to characterize the electronic properties of this material in more detail and to determine its band structure the preparation of azimuthally well defined possibly epitaxially ordered films is desirable. Previous attempts have shown that in contrast to pentacene films which grow epitaxially on Bi(0001)/Si such an ordering does not occur for PFP [3]. In this study we compare the structure and morphology of PFP-films grown by OMBD onto SiO2, sapphire and various alkali halide surfaces which have been characterized by AFM, XRD, FTIR and TDS. It is shown that on some alkali halide surfaces uniformly oriented PFP-islands are formed which reflects an epitaxial ordering. The different film structures are discussed in terms of template induced film growth.

[1] Suzuki et al., J. Am. Chem. Soc., 126, 8138 (2004)
[2] Kowarik et al., phys. stat. sol. (RRL) 2, 120 (2008)
[3] Wang et al., Nanotechnology 20, 095704 (2009)

DS 29.13 Wed 15:00 Poster A

Conductivity improvement of graphite-like ion tracks in tetrahedral amorphous carbon — •Anne-Katrin Nix[1], Hans-Gregor Gehrke[1], Johann Krauser[2], Christina Trautmann[3], Alois Weidinger[4], and Hans Hofsäss[1] — [1]II. Physikalisches Institut, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany — [2]Hochschule Harz, University of Applied Sciences, 38855 Wernigerode, Germany — [3]GSI Helmholtzzentrum für Schwerionenforschung, Planckstraße 1, 64291 Darmstadt, Germany — [4]Helmholtz-Zentrum Berlin für Materialien u. Energie, 14109 Berlin, Germany

The irradiation of insulating tetrahedral amorphous carbon (ta-C) with swift heavy ions leads to creation of conductive ion tracks of 8 nm diameter and length depending on the film thickness. Our recent studies show that the track conductivity increases in ta-C layers of lower sp^3 bond content, which in turn increases the overall conductivity of the surrounding matrix. To improve the track conductivity and retain the insulating properties of ta-C, two approaches were made. First, doped ta-C films were prepared by mass selected ion beam deposition, together with iron or nitrogen as a dopant. These few impurities in the matrix are expected to improve the ion track conductivity by increasing the number of hopping sites because the conduction process is known to be dominated by variable-range hopping. Second, ta-C samples were irradiated with C_{60} projectiles, which have a much higher energy loss than monoatomic projectiles, and thus form larger and more conductive tracks.

DS 29.14 Wed 15:00 Poster A

Rekristallisation von a-Si– und a-Ge–Nanostrukturen — •Jens Bauer, Chinmay Khare, Michael Weise und Bernd Rauschenbach — Leibniz-Institut für Oberflächenmodifizierung, Permoserstrasse 15, D-04318 Leipzig, Germany

Die Glanzwinkelabscheidung (GLAD: „glancing angle deposition“) stellt eine spezielle Methode der physikalischen Gasphasenabscheidung von porösen Schichten dar. Dabei erreicht der einfallende Partikelfluss die Substratoberfläche unter streifendem Einfallswinkel (üblicherweise $< 5°$). Bereits im Bereich der Anfangsabscheidung schatten sich benachbarte Strukturen aufgrund dieses extrem flachen Partikeleinfallswinkels gegenseitig ab. Das resultierende konkurrierende Wachstum führt zur Ausbildung einer definierten Nanostruktur aus geneigten Nadeln, die in Richtung des einfallenden Partikelflusses orientiert vorliegen. Durch zusätzliche Substratrotation lässt sich die Nanostruktur gezielt variieren. So lassen sich bspw. Nanospiralen, -schrauben oder senkrechte Nanosäulen realisieren, die wiederum aus nanoskopischen Fasern (d=20-30 nm) bestehen. Im Beitrag stellen wir Ergebnisse zur GLAD-Herstellung von nanostrukturierten a-Si– und a-Ge–Schichten vor. Im Vergleich zu kompakten a-Si– und a-Ge–Volumenmaterialschichten wurde die Rekristallisation im Temperaturbereich von RT–1200°C untersucht. Der Einfluss von Temperatur und Annealingzeit werden auf Grundlage von Röntgenbeugungsexperimenten diskutiert.

DS 29.15 Wed 15:00 Poster A

Growth of crystalline Ag nanorods by ion beam sputter glancing angle deposition — •Chinmay Khare[1], Christian Patzig[1], Jürgen. W Gerlach[1], Bodo Fuhrmann[2], Hartmut. S Leipner[2], and Bernd Rauschenbach[1] — [1]Leibniz-Institut of Surface Modification, Permoserstraße 15, 04318 Leipzig, Germany — [2]Martin-Luther-University Halle, Heinrich-Damerow-Straße 4, 06120 Halle, Germany

Glancing angle deposition (GLAD) is an efficient physical vapour deposition process to sculpt columnar nanostructures. When the particle flux reaches the substrate under a highly oblique angle β (β * 80°, as measured to the substrate normal), inherent self-shadowing mechanism causes growth of needle-like structures. Here, ion beam sputter glancing angle deposition of Ag nanostructures with different morphologies on planar and pre-patterned substrates either at room temperature (RT) or elevated substrate temperatures are demonstrated. Randomly distributed nanostructures are observed on planar substrates, while patterned templates with different periodicity yield growth of well organised periodic structures at RT. A broad angular divergence of the sputtered particle flux is minimised by a slit aperture. At room temperature, columnar structures are observed, irrespective of the presence of the slit aperture. At elevated temperatures (300°C, 350°C) and collimated particle flux in the presence of the slit aperture, however, accelerated surface diffusion causes the growth of crystalline nanorod- and nanowire-like structures. In the absence of the slit aperture, the particle beam divergence is higher, leading to island- and mountain-like crystalline structures that are found at elevated temperatures.

DS 29.16 Wed 15:00 Poster A

IR studies on the interaction of Ca and Mg with the blue emitter material Ir(cn-pmbic)$_3$ — •Tobias Glaser[1], Martin Binder[1], Annemarie Pucci[1], Christian Lennartz[2], and Christian Schildknecht[2] — [1]Kirchhoff-Institut für Physik, Universität Heidelberg, INF 227, 69120 Heidelberg — [2]BASF SE, 67056 Ludwigshafen

Ca and Mg play an important role as cathode materials in organic light emitting devices (OLEDs). The interaction of these metals with the blue phosphorescent emitter material Ir(cn-pmbic)$_3$ is investigated by infrared (IR) spectroscopy. Thin films of the organic material are deposited by vapour sublimation on a gold substrate under UHV conditions. The deposition of Ca on the organic layer gives rise to new features in the IR-spectrum of the sample. These new features are supposed to be related to dynamic charge transfer processes. On the other hand, Mg does not seem to form a conducting layer on the organic material.

DS 29.17 Wed 15:00 Poster A

Modification of Au and Si(111):H Surfaces towards Biological Sensing — •Xin Zhang[1], Guoguang Sun[2], Karsten Hinrichs[2], Dana Rosu[2], Norbert Esser[2], Marc Hovestaedt[3], Bernhard Ay[3], Rudolf Volkmer[3], Silvia Janietz[4], and Jörg Rappich[1] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Institut für Si Photovoltaik, Berlin, Germany — [2]2 ISAS-Institute for Analytical Sciences, Department Berlin, Germany — [3]3 Institut für medizinische Immunologie, Charité Berlin, Berlin, Germany — [4]4 Fraunhofer-Institut für Angewandte Polymerforschung, Golm, Germany

Within the topics to grow functional organic surfaces for biosensors we grafted carboxylbenzene, aminobenzene and maleimidobenzene onto Au and H-terminated Si surfaces by electrochemical deposition from 4-carboxylbenzene-diazonium tetrafluoroborate (4-CBDT), 4-aminobenzene-diazonium tetrafluoroborate (4-ABDT) and 4-maleimidobenzene-diazonium tetrafluoroborate (4-MBDT).The electron injection to the diazonium compound in solution (cathodic current) leads to the formation of intermediate radicals, which further react with the surface (Au or Si:H) and the respective molecule is grafted onto the surface.The aim was to functionalise these surfaces for further reaction with corresponding amines, acids or cysteine-modified peptides. Ex-situ infrared spectroscopic ellipsometry (IRSE) was applied to inspect the surface species before and after the functionalisation.

DS 29.18 Wed 15:00 Poster A

Infrared spectroscopic ellipsometry of organic semiconductor layers — •Robert Lovrinčić, Jens Trollmann, and Annemarie Pucci — Kirchhoff-Institut für Physik der Universität Heidelberg

Organic semiconductors are very interesting for many applications as they are printable on a variety of substrates in large areas and at low costs. Within the production process many steps are necessary which might influence the chemical composition of the material and thereby the electrical performance of the device. Chemical information can be obtained from spectroscopic measurements in the mid infrared (fingerprint region).

We perform variable angle infrared spectroscopic ellipsometry to determine the dielectric function of organic semiconductor layers in the spectral region $350 - 5000\,\mathrm{cm}^{-1}$ by means of a commercial IR-ellipsometer (Woollam IR-VASE). The anisotropy of the resulting dielectric function will be discussed. Moreover, by changing the sample temperature during measurement the stability of the semiconductor can be investigated.

DS 29.19 Wed 15:00 Poster A

Optical properties of single crystalline silicon nanowires — •Gerald Brönstrup and Silke Christiansen — Institut für Photonische Technologien e.V., Abt. Halbleiter-Nanostrukturen, 07745

Jena

Silicon Nanowires [SiNWs] have attracted much attention in the recent years as possible future building blocks for field effect transistors, sensors, solar cells and photo detectors. However an analysis of the optical properties of single SiNWs has not been published to the best of our knowledge. Here we present a theoretical analysis using the well known Mie-theory. We calculated the absorption and scattering cross sections with respect to the radius of the SiNWs the angle of incident of the illuminating light, its polarization and wavelength. In the limit of ray optics the cross sections are limited to the geometrical area of the illuminated objects. Since the dimensions of SiNWs can be much smaller than the wavelength of the visible light, ray optics cannot be used. Because of that and the wave nature of light the cross sections could be larger than the geometrical area of the SiNWs. Indeed we found that both scattering and absorption cross sections are much larger than the geometrical area of the SiNW for certain wavelengths and radii. Additionally a strong dependence on both the radii of the SiNWs and the wavelength of the illuminating light was found. This makes it possible to tune future devices to certain wavelengths by synthesizing SiNWs with the appropriate radius.

DS 29.20 Wed 15:00 Poster A

Terahertz Plasmon Dispersion Relation in Layered Semiconductor Structures — •Daniel Dietze, Juraj Darmo, and Karl Unterrainer — TU Wien, Institut für Photonik, 1040 Wien, Österreich

Surface guided waves, so-called plasmons, have attracted considerable attention in the past years due to their possible use for sub-wavelength confinement and guiding of terahertz (THz) electromagnetic fields [1]. Fundamental insight into the behavior of plasmons can be obtained from their dispersion relation, which links the in-plane wave vector β to the angular frequency ω. In general, the underlying equations are transcendental and stability of the numerical methods becomes an issue in the THz spectral range, as the characteristic frequencies are often separated by orders of magnitude.

In our contribution, we present a robust method which does not require any prior knowledge about the dispersion relation or the mode structure. It is based on simplex minimization in three dimensions, a Monte-Carlo approach for the initial values and analytical expressions for the transcendental equations. Additionally, we included the possibility of conducting interfaces, which allows modeling of systems including 2DEG layers, such as HEMTS or graphene based devices. Several examples are presented which are of current technological interest.

[1] J. A. Dionne, L. A. Sweatlock, H. A. Atwater, and A. Polman, Phys. Rev. B **73**, 035407 (2006)

DS 29.21 Wed 15:00 Poster A

Space charge effects and charge injection in organic semiconductors — •Marlis Ortel, Sidhant Bom, Torsten Balster, Benedikt Gburek, and Veit Wagner — School of Engineering and Science, Jacobs University Bremen, Campus Ring 1, 28759 Bremen, Germany

Organic circuits with high-frequency switching properties are important for an increasing number of applications. It has been shown that contact resistance sets a limit towards higher frequencies.1 Therefore it is crucial to obtain good injection properties of charge carriers from the contact materials into the organic semiconductor.

It is known that injection of charge carriers is influenced by space charges at the interface caused by low mobilities of semiconducting materials. For different transport mechanisms possible in organic semiconductor materials different forms of space charge zones can be predicted by theory close to the injecting contact.

Experimentally current-voltage measurements are performed on various thiophene-based devices. The investigated thiophene-based materials are selected such, that they realize strongly different transport behavior. The measurements are compared to the theoretical predictions. We find, that higher disorder results in a larger space charge region even for the same mobility value.

1 V. Wagner, P. Wöbkenberg, A. Hoppe, J. Seekamp; Appl. Phys. Lett. 89 (2006) 243515.1-3

DS 29.22 Wed 15:00 Poster A

Waveguide and surface plasmon losses in organic light-emitting diodes (OLED's) — •Bert Scholz, Jörg Frischeisen, and Wolfgang Brütting — Institute of Physics, University of Augsburg, Germany

As a new technology in light sources the organic light-emitting diodes (OLEDs) have improved rapidly in recent years. One of the remaining challenges is to enhance light outcoupling. Especially the excitation of waveguide modes (WGMs) inside the organic layers and surface plasmons (SPs) at the interface to the cathode strongly reduce the efficiency. These loss channels usually are not accessible for a profound analysis. Therefore, we investigate a simplified OLED stack consisting of only a glass substrate, a metallic silver layer and Alq$_3$ (tris-(8-hydroxyquinoline) aluminum). In this stack it is possible to extract and measure WGMs as leaky modes and to couple out SPs by a reversed Kretschmann configuration. The occurrence and extraction of WGMs and SPs is studied in detail by varying the thickness of the silver and the Alq$_3$ layer and by a comparison to numerical simulations. The results obtained in this study offer a deeper understanding of WGMs and SPs, which is a first step to reduce these optical losses and to significantly enhance the efficiency of OLEDs.

DS 29.23 Wed 15:00 Poster A

Simulation of outcoupling efficiencies of OLEDs — •Richard Pfeifer^1, Beatrice Beyer^1, Karsten Fehse^1, and Karl Leo^{1,2} — ^{1}Fraunhofer IPMS, Dresden, Germany — ^{2}Institut für Angewandte Photophysik, TU Dresden Germany

Organic light-emitting diodes (OLEDs) are now commercially available in various lighting and display applications. While their electrical and optical properties have been greatly improved by the use of pin-OLEDs, the external quantum efficiency is still limited by the relative low outcoupling efficiency of the generated radiation of 20-25%. To address this field of light outcoupling improvement, we use a simulation based on the freely available open-source-framework CAMFR [1] to calculate the optical properties of planar top-emitting-OLEDs, i.e their angle dependent spectra and the total outcoupling efficiency and compare our results to experimental data. The simulation focus is put on the power distribution of the radiating dipoles into different decay channels as outcoupling modes, guided modes, surface-plasmon modes, and absorption losses. Calculation of these relative contributions enables us to identify the main loss channels of radiated power. Together with the potential of the CAMFR-framework to calculate multilayer systems with periodically structured layers, the optimization of light-outcoupling by integration of diffractive periodic structures is discussed.

[1] P. Bienstman, R. Baets, Optical and Quantum Electronics, 33, p.327-341 (2001)

DS 29.24 Wed 15:00 Poster A

Investigation of degradation phenomena of blue fluorescent OLEDs — •Ruben Seifert, Sebastian Scholz, Björn Lüssem, and Karl Leo — Institut für Angewandte Photophysik TU Dresden, D-01062 Dresden

During the last years, the lifetime of organic light emitting diodes (OLEDs) based on small molecules has greatly improved. However, there are still problems concerning the long term stability of blue emitters. In this contribution, we describe experiments on p-i-n bottom emitting OLEDs with the blue emitting substance Spiro-DPVBi (2,2',7,7 tetrakis (2,2diphenylvinyl)-spiro-9,9'-biuoren). It is known that the main intrinsic degradation process of Spiro-DPVBi is not influenced by the electric current or the applied field, but it has been proposed that the degradation is caused by the exciton density [1]. To prove this, we did experiments on hole- and electron-only devices with very high charge carrier densities. To investigate the influence of excitons on degradation, we compare an electrical and an UV-aged OLED with the same initial luminance. Since Spiro-DPVBi is an efficient fluorescent material, the UV-radiation is creating singlet excitons only. However, both samples show similar degradation behavior, so that we can assume that the degradation of Spiro-DPVBi is mainly caused by singlet excitons.

[1] Winter, S., Reineke, S., Walzer, K., Leo, K., Proc. of SPIE Vol.6999, 69992N-8 (2008).

DS 29.25 Wed 15:00 Poster A

Integration of non-volatile organic memory devices and organic diodes into a passive matrix crossbar array — •Philipp Sebastian, Hans Kleemann, Björn Lüssem, and Karl Leo — Institut für Angewandte Photophysik, TU Dresden, Germany

Within the last few years organic memory devices have attracted considerable attention. Several different approaches for organic memory devices have been reported in literature. Some of them show remarkable device performance regarding the ON/OFF ratio and switching speed [1]. However, besides optimizing the performance of a single memory cell, it is further necessary to integrate the memory cell in a crossbar structure of top and bottom contacts to address the device properly and obtain high data storage density [2]. To avoid unwanted crosstalk between neighbouring elements in a passive matrix, the resistive memory element has to be combined with an organic diode. Here, we report on an approach to integrate an organic memory device [3] stacked with an organic diode element into a passive matrix structure. It is shown that the combination of an organic memory and a rectifying diode efficiently suppresses crosstalk in the crossbar. In order to increase the possible size of the crossbar array, the rectification ratio and the maximum forward current of the diode is increased. Furthermore, by optical lithography the possible integration density is raised.

[1] J. Scott, L. Bozano, Advanced Materials 19, 1452 (2007) [2] E. Teo et al., IEEE Electron Device Letters 30, 487 (2009) [3] F. Lindner, K. Walzer, K. Leo, Applied Physics Letters 93, 233305 (2008)

DS 29.26 Wed 15:00 Poster A

Influence of substrate charge on organic field effect transistors — •Lorenz Kehrer, Christian Melzer, and Heinz von Seggern — Electronic Materials Department, Institute of Materials Science, Technische Universität Darmstadt, Petersenstraße 23, 64287 Darmstadt, Germany

The development of printed electronics on flexible substrates is a great challenge for current research. During a continuous roll-to-roll process the often used plastic substrate can be unintentionally charged by contact electrification or by a controlled corona discharge to improve the adhesion of the organic inks. It is thus worth investigating the time and temperature stability of the trapped substrate charge and the impact of the remaining charge on the device operation. We have investigated the charging process of PET by applying different corona charging conditions and by detecting the resulting surface potential with a Kelvin probe as a function of time and temperature following the charging procedure. By measuring thermal stimulated currents the trap distribution as well as the thermal and temporal stability of the substrate charge was analyzed. The effects of existing substrate charge on a top gate organic field effect transistor is discussed and further simulated by dual gate transistors with well defined electrode potentials.

DS 29.27 Wed 15:00 Poster A

Charge transport across Zinc Oxide Field Effect Transistors — •Daniel Walker, Christopher Siol, Christian Meltzer, and Heinz von Seggern — Electronic Materials Department, Institute of Materials Science, Technische Universität Darmstadt, Petersenstraße 23, 64287 Darmstadt, Germany

Zinc-Oxide is a highly attractive material for next generation electronic products as it is low cost and exhibits n-type semi-conducting properties and thus can be used in the fabrication of thin film field effect transistors; however the mechanism underlying the electronic behaviour remains poorly understood. This poster will present work examining the charge flow through spin coated Zinc-oxide FET by measurement of the surface potential using an ultra high-vacuum Kelvin-Probe force microscopy technique combined with a conventional voltage-current characterisation of the FET. A typical potential drop from the source to drain has been observed and is presented as a surface potential profile related to the position in the channel. Furthermore topographic data will be presented alongside a surface potential map in order to discern the effects of surface features on the charge-transport properties.

DS 29.28 Wed 15:00 Poster A

Optimized Adsorption of Sulfonated Phthalocyanines on ZnO Electrodes and Their Characterization in Dye- Sensitized Solar Cells — •Jane Falgenhauer, Thomas Loewenstein, and Derck Schlettwein — Institute of Applied Physics, Justus-Liebig-University Giessen, Germany. email:schlettwein@uni-giessen.de

Phthalocyanines belong to the most stable industrial dyes and show some of the highest molar extinction coefficients in the visible range. ZnO is known as a wide band gap semiconductor material which can be conveniently prepared as a porous electrode from solution-based processes. Sulfonated phthalocyanines were adsorbed at such electrodeposited porous ZnO thin films to work as a photosensitizer in a dye sensitized solar cell (DSSC). The adsorption solution of the phthalocyanine was modified in its composition and by adding different detergents in different concentrations. The adsorption solutions and the sensitized ZnO films were investigated by UV/Vis spectroscopy to characterize the aggregation of the dye molecules. Most of the detergents used could minimize the aggregation of the dye molecules in the adsorption solution without hindering the adsorption of the phthalocyanine on the ZnO surface. The photoelectrochemical characteristics of the resulting test cells were determined using a standard liquid electrolyte. The efficiency of the cells did not reach the expected level and reasons for this are discussed based on film morphology, amount of adsorbed dye molecules, competition by detergent adsorption, the optical absorbance of the dyes in the film and aggregate formation.

DS 29.29 Wed 15:00 Poster A

DIP based organic photovoltaic cells with high fill factor and high open circuit voltage — •Mark Gruber, Julia Wagner, Andreas Opitz, and Wolfgang Brütting — Institute of Physics, University of Augsburg, Germany

The p-type semiconductor Diindenoperylene (DIP) was used as a donor material in combination with the acceptor C_{60} for the application in planar and bulk heterojunction organic solar cells. The favourable molecular energy level alignment mainly affected by the low lying HOMO of DIP results in high open circuit voltages of up to 0.94 V under 100 mW/cm^2 simulated AM1.5 illumination. DIP shows comparatively low absorption coefficients which can be attributed to predominantly upright standing molecules leading to unfavourable orientation of the optical transition dipole. Nevertheless, the high open circuit voltages together with remarkably high fill factors of around 74% - approaching those of silicon solar cells show great promise for highly efficient photovoltaic cells.

Morphological investigations demonstrate strong dependence of the growth behaviour on substrate temperature. By varying the growth conditions large variations in crystallinity are observed and are related to solar cell performance. Thus, dependent on the substrate temperature the shape of the current-voltage curve changes from distinct s-shape to nearly perfect diode characteristics.

DS 29.30 Wed 15:00 Poster A

In-situ Characterization of Evaporated Organic Bulk Heterojunctions During Their Film Growth — •Max Beu, André Dragässer, Christopher Keil, and Derck Schlettwein — Institute of Applied Physics, Justus-Liebig-University Giessen, Germany. email:schlettwein@uni-giessen.de

Vapor deposited heterojunction thin films of C_{60} and $CuPc$ in the low nanometer range on glass substrates were studied in-situ by measuring their thickness-dependent current-voltage characteristics at various illumination wavelengths and light intensities. The film growth was investigated under the influence of different substrate temperatures, polarizing voltages and illumination conditions. Consequences for the photoconductivity of the composites were determined. Charge transfer among the constituents is discussed as a basis for their use as photovoltaic junction materials.

DS 29.31 Wed 15:00 Poster A

Interface properties and electronic structure of PCPDTBT - a promising polymer for organic solar cells — Umut Aygül, •Fotini Petraki, Holger Hintz, Heiko Peisert, and Thomas Chassé — Institute of Physical and Theoretical Chemistry, University of Tübingen, Germany

Mankind's energy demand is steadily increasing. Novel techniques for environmental friendly energy conversion are therefore a challenging task. Organic solar cells based on donor-acceptor blends present a quite new approach, which posses a large market potential although their efficiency is rather low compared to their inorganic counterparts. In polymer based "bulk heterojunction"-type solar cells so-called "low bandgap" materials are promising donor components in active layers. Low optical bandgap conjugated polymers may improve the efficiency of organic photovoltaic devices by increasing the absorption in the visible and near infrared region of the solar spectrum and by optimizing the offset of the LUMO (lowest unoccupied molecular orbital) energy levels of the donor and acceptor. 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). We study the electronic structure and interface properties to gold and ITO of PCPDTBT by X-ray and UV photoemission spectroscopies (XPS, UPS) as well as X-ray absorption spectroscopy (XAS). The energy level alignment points to charge transfer processes across the interface. In addition, strong chemical interactions occur which may have consequences for interface properties in devices.

DS 29.32 Wed 15:00 Poster A

relationship between the morphology and charge transport in the hybrid system composed of conductive polymer and CdSe nanoparticles — •nikolay radychev, irina lokteva, joanna kolny-olesiak, elizabeth von hauff, holger borchert, and jürgen parisi — Institute of Physics, Energy and Semiconductor Research Laboratory, University of Oldenburg,Oldenburg,Germany

Hybrid systems based on a bulk heterojunction of conductive polymer and semiconductor nanoparticles is one of the promising approaches for low cost and printable solar cell fabrication. However the light conversion efficiencies of these systems are quite low (~2-3 percent) compared to inorganic solar cells. One limiting factor in the organic-inorganic hybrid solar cells is the comparably low charge carrier mobility which impedes efficient charge transport. Furthermore, the morphology of the active layer is difficult to control which contributes to limited light conversion efficiency as well. In the present work, composites of poly(3-hexylthiophene) and colloidally synthesized CdSe nanoparticles were prepared. The nanoparticles possess an organic ligand shell after synthesis which needs to be replaced by pyridine prior to use in solar cells. The influence of the ligand exchange on the active layer morphology was investigated here. Charge carrier mobility was investigated by OFET methods. The results were compared with a theoretical model based on the fitting of the current-voltage characteristics. Relationships between the morphology and charge transport were analyzed.

DS 29.33 Wed 15:00 Poster A

Changes in inorganic matricees of dye sensitized solar cells during preparation — •Harald Graaf[1], Carsten Maedler[1,2], Thomas Baumgärtel[1], Franziska Lüttich[1], Mirko Kehr[1], and Thorsten Oekermann[3] — [1]Institute of Physics, University of Technology Chemnitz, 09107 Chemnitz, Germany — [2]Department of Physics, Boston University, Boston, MA 02215, USA — [3]Institute of Physical Chemistry and Electrochemistry, Leibniz University Hannover, 30167 Hannover, Germany

Dye-sensitized solar cells (DSSC) containing zinc oxide (ZnO) as the inorganic semiconductor and organic dye molecules as the sensitizer are well known devices with high efficiency. Such DSSC are prepared by electrochemical deposition of an aqueous zinc salt solution including organic molecules as templates. The template is desorbed in a second step to obtain a porous ZnO network. As a final step the senzitizing organic molecules were re-adsorped from solution. Within these different processing steps the structure of the ZnO can be influenced. We will discuss the growth mechanism during film deposition e.g. due to different template molecules. Also the crystal structure changes accompanying the desorption process, which is performed in an alkaline aqueous solution. Different techniques as X-ray investigations, optical absorption and scanning probe methods are used to identify the variations in different cells and within the production process.

DS 29.34 Wed 15:00 Poster A

Controlling the energy levels at interfaces between conjugated organic materials and electrodes — •Benjamin Bröker[1], Ralf-Peter Blum[1], Georg Heimel[1], Johannes Frisch[1], Jürgen P. Rabe[1], Antje Vollmer[2], Oliver T. Hofmann[3], Egbert Zojer[3], Ralph Rieger[4], Klaus Müllen[4], and Norbert Koch[1] — [1]Institut für Physik, Humboldt-Universität zu Berlin, D-12389 Berlin, Germany — [2]Helmholtz-Zentrum Berlin für Materialien und Energie -Bessy II, D-12489 Berlin, Germany — [3]Institut of Solid State Physics, Graz University of Technology, A-8010 Graz, Austria — [4]Max Planck Institut für Polymerforschung, D-55128 Mainz, Germany

In the past decades, the field of organic electronics has made tremendous progress, which led to significant increase in device performance. However, the interfaces between the electrodes and the conjugated organic material (COM) can still be identified as one of the key areas for device improvement. Several strategies towards adjusting the electronic levels of the electrode-COM interface exist, with one of them being the adsorption of molecules that undergo a charge-transfer-type reaction with the electrode materials. This modifies the energy level alignment and leads to significantly decreased injection barriers for subseqently deposited COM layers. In this work we present an overview of donor and acceptor molecules. By application of thin layers of these molecules a tunability of the substrate work function over a range of almost 3eV was achieved. Furthermore a variety of electronic as well as structural phenomena were identified at these interfaces that can play an important role in the charge injection process.

DS 29.35 Wed 15:00 Poster A

Interface recombination effect in modelling the photoelectrical characteristics of P3HT:PCBM bulk heterojunction solar cells — •Jędrzej Szmytkowski — Institut für Angewandte Physik, Universität Karlsruhe (TH), Karlsruhe, Germany

The interface recombination of charge carriers located in the material with lower permittivity [1] has been implemented for the first time to calculate the electrical characteristics of donor–acceptor P3HT:PCBM bulk heterojunction solar cell. In order to estimate the photocurrent density in this system, a simple analytical formula has been derived. Theoretical I–V characteristics agree well with experimental data obtained in different laboratories. The conclusion is that the major contribution to the recombination in P3HT:PCBM blend is from the interface recombination with negligible contribution from the Langevin–type recombination. However, other processes could be also taken into account to explain the reduction of Langevin–type recombination. We suggest that the Braun–Onsager model cannot be used in the case when both materials in the blend are characterized by different permittivities.

[1] J. Szmytkowski *Chem. Phys. Lett.* **470** (2009) 123

DS 29.36 Wed 15:00 Poster A

Correlation of morphology, cell architecture and device performance in P3HT/fullerene based organic solar cells — •Ulrich Hörmann[1], Julia Wagner[1], Andreas Opitz[1], Wolfgang Brütting[1], and Ellen Moons[2] — [1]Institute of Physics, University of Augsburg, Germany — [2]Department of Physics, Karlstad University, Sweden

The material combination of the polymer poly(3-hexylthiophene) (P3HT) and the fullerene derivative [6,6]-phenyl-C_{61}-butyric acid methyl ester (PCBM) is one of the most widespread donor-acceptor systems in organic photovoltaics. In the present work these materials as well as the buckminsterfullerene C_{60} are studied in three different device architectures: the bulk heterojunction, the planar heterojunction and the diffuse heterojunction, which can be considered as a combination of both.

Planar heterojunctions are achieved by evaporation of either C_{60} or PCBM onto a spin-coated P3HT layer. Heating the P3HT film to an appropriate temperature during the evaporation process enables the C_{60} molecules to penetrate into the polymer layer, representing a new technique of producing diffuse donor-acceptor interfaces. Preparation of diffuse heterojunctions with PCBM can be achieved by means of spin coating while partly dissolving the underlying P3HT. Morphological investigations of the resulting layers have been performed by scanning force microscopy as well as optical and fluorescence microscopy and emphasize the importance of morphology and device architecture for the performance of organic photovoltaic cells.

DS 29.37 Wed 15:00 Poster A

Investigation and Control of the Nanomorphology in Solution Cast Thin Polymer-Fullerene P3HT:PCBM Films — •Benedikt Brenneis[1], Benjamin Schmidt-Hansberg[1], Monamie Sanyal[2], Esther Barrena[2], Michael Klein[3], Philip Scharfer[1], Dagmar Gerthsen[4], and Wilhelm Schabel[1] — [1]KIT Thermal Process Engineering / Thin Film Technology, Karlsruhe, Germany — [2]Max Planck Institute, Stuttgart, Germany — [3]KIT Light Technology Institute, Karlsruhe, Germany — [4]KIT Laboratory for Electron Microscopy, Karlsruhe, Germany

In this work we investigate the drying process of solution cast thin polymer-fullerene films with respect to the interplay of process conditions and device properties. The established material system P3HT:PCBM for organic photovoltaic devices is solution cast and subsequently dried under several drying conditions varying the drying temperature, the drying air flow speed in a drying channel and other coating properties. By using atomic force microscopy (AFM), grazing incidence x-ray diffraction (GIXRD), scanning transmission electron microscopy (STEM) and more utilities the film morphology and optoelectronic properties are investigated systemically and correlated with the film formation history.

DS 29.38 Wed 15:00 Poster A

In-situ AFM study of P3HT:PCBM mixtures during thermal annealing — •Abel Roigé[1], J. Oriol Ossó[1], Malte Schmidt[2], and Mariano Campoy-Quiles[2] — [1]MATGAS 2000 AIE, Campus de la UAB — [2]Institut de Ciència de Materials de Barcelona, CSIC

Polymer-small molecule donor-acceptor blends are currently being extensively investigated due to their use as photovoltaic materials. Postdeposition annealing treatments have proven to be one of the most effective methods to enhance organic solar cell performance. One of the main changes experienced by the materials during heating is the self-assembly of polymer chains which induces an increase in charge transport and light absorption. However, the particular changes and concomitant device improvements strongly depend on the specific processing conditions. It is, thus, clear, that novel ways of monitoring the morphological changes associated to these treatments can be strongly beneficial for the optimization of organic solar cells. In this work, we use in-situ AFM measurements to detect changes in topography and surface roughness upon heating for the workhorse material system (P3HT:PCBM). These measurements allow to visualize the polymer crystallization at 140°C as well as a clear decrease in roughness at around 100°C. In addition, in-situ Raman spectroscopy experiments and conductive AFM complement real time topographical data to detect the structural changes that occur during annealing and their effect on the electric transport properties. The combination of these techniques allows a detailed characterization of the morphological changes that organic materials undergo during thermal annealing.

DS 29.39 Wed 15:00 Poster A

Conductive Atomic Force Microscopy Investigations of Organic thin Films — •Andreas Pavitschitz[1], Igor Beinik[1], Markus Kratzer[1], Christian Teichert[1], Simone-Viola Radl[2], Thomas Griesser[2], and Wolfgang Kern[2] — [1]Institute of Physics, University of Leoben, 8700 Leoben, Austria — [2]Institute of Chemistry of Polymeric Materials, University of Leoben, 8700 Leoben, Austria

Organic materials are used in electronic devices as dielectrics, semiconductors and conductive materials. The device performance depends on the electrical properties and the surface morphology of the organic thin film. Conductive Atomic Force Microscopy (C-AFM) allows simultaneous mapping of the morphology and the local film conductivity on the nanometer-scale. Access to details of carrier transport can be obtained by measuring local current - voltage (I/V) curves. In this study, C-AFM was used to investigate a UV sensitive conductive polymer. The polymer layers were prepared by spin coating on Au/glass and ITO. C-AFM proved a increase in conductivity in the polymer film after UV-exposure.

Support by the FWF projects S9702 N- 20, S9707 and P19636 is acknowledged.

DS 29.40 Wed 15:00 Poster A

Influence of Auxiliary Plasma Source on Properties of Photoactive TiO2 Films by MePIII&D — •Altin Gjevori[1,2], Dietmar Hirsch[1], Jurgen W. Gerlach[1], Darina Manova[1], and Stephan Mändl[1] — [1]Leibniz-Institut für Oberflächenmodifizierung, 04318 Leipzig, Germany — [2]Faculty of Natural Sciences, University of Tirana, Tirana, Albania

For several years, TiO2 is receiving increasing scientific attention as one of the most promising photo catalysts with a huge potential for solving several different types of environmental problems. While TiO2 powders and nanoparticles are well known and widely used, thin film surfaces are less investigated but still highly desired for applications. For TiO2 polymorphs, anatase powder is reported to be a more potent photo catalyst than rutile. Metal plasma immersion ion implantation and deposition is employed to form titanium oxide films at room temperature. By applying high voltage pulses of up to 5 kV at a duty cycle of 30%, polycrystalline films could be obtained. Additionally, an RF plasma source was used to increase the ionisation of the background oxygen gas at different flow rates, thus enhancing the ion bombardment of the surface. AFM, SEM, XRD and surface energy measurements show that by employing the auxiliary RF plasma source, a lower oxygen gas flux is compensated by increasing the oxygen content compared to the case without auxiliary plasma.

DS 29.41 Wed 15:00 Poster A

Formation of palladium hydrides in low temperature Ar/H$_2$-plasma — •Harm Wulff, Marion Quaas, Heiko Ahrens, Oxana Ivanova, and Christiane A. Helm — University of Greifswald, Institute of Physics, F.-Hausdorff-Str. 6, 17487 Greifswald

A specific challenge in low temperature plasma science is the investigation of chemical reactions in solid surface layers as a response to external plasma parameters.

20 nm thick palladium films were exposed to argon-hydrogen microwave plasma using different negative substrate voltages to study the hydride formation. The palladium hydride films were investigated by grazing incidence x-ray diffractometry (GIXD, Hasylab, Hamburg - Surface layers in reactive plasmas - project I-20080137)), in-situ high temperature x-ray diffractometry (HT-GIXD), x-ray reflectometry (XR) and atomic force microscopy (AFM).

The effect of hydrogen plasma depends on the applied negative bias voltage. Up to -50 V we observe an increase of the fcc Pd unit cell volume. Hydrogen atoms occupy octahedral interstices to form PdH$_{0.55}$. However, bias voltages of -100 V and -150 V cause a shrinking of the fcc Pd unit cell in two steps to fcc Pd$_{VacI}$ and fcc Pd$_{VacII}$. Subsequent reactions under long time plasma exposure form cubic PdH$_{1.33}$. HT-GIXD experiments confirm the existence of different palladium hydrides. PdH$_{0.55}$ lost its hydrogen at temperatures $>$ 600 K. From the phase transformations PdH$_{1.33}$ ($>$ 700 K) –> Pd$_{VacII}$ (1000 K) –> PdH$_{1.33}$ we draw the conclusion that Pd$_{Vac}$ is a hydride compound. The formation mechanisms of palladium hydrides will be discussed.

DS 29.42 Wed 15:00 Poster A

Complementary ion beam analysis and photo electron spectroscopy study of oxygen contamination in epitaxial GdN films on YSZ substrates — •Jürgen W. Gerlach[1], Walter Assmann[2], and Bernd Rauschenbach[1] — [1]Leibniz-Institut für Oberflächenmodifizierung, 04318 Leipzig — [2]Ludwig-Maximilians-Universität München, Maier-Leibnitz-Laboratorium, 85748 Garching

Gadolinium nitride (GdN) is a ferromagnetic material with a Curie temperature at 75 K and with promising electronic properties. In the present study, the low-energy ion-beam assisted epitaxial growth of thin GdN films on yttria-stabilized zirconia (YSZ) substrates is investigated. For this purpose, Gd was deposited on the substrate and simultaneously irradiated with a hyperthermal nitrogen ion beam at a constant substrate temperature of 750°C. To prevent rapid oxidation of GdN in air, a GaN protective layer was deposited. According to x-ray diffraction (XRD), the formation of epitaxial GdN on YSZ(100) was achieved, but time-of-flight secondary ion mass spectrometry (TOF-SIMS) showed that first a gadolinium oxide layer was formed and during further deposition the GdN phase was dominating over the still coexisting oxide. This was confirmed by quantitative elastic recoil detection analysis (ERDA) exhibiting a high degree of oxygen contamination over the whole film thickness. The chemical nature of the contamination was assessed by photo electron spectroscopy (XPS). It could be excluded that the oxygen contamination originated from residual gases in the ultra-high vacuum recipient. Instead, the oxygen was found to diffuse from the YSZ substrate into the GdN film.

DS 29.43 Wed 15:00 Poster A

X-ray Photoelectron Diffraction of Perovskite Oxides — •Mathias Glaser, Christoph Raisch, and Thomas Chassé — Universität Tübingen, Institut für Physikalische und Theoretische Chemie, Auf der Morgenstelle 8

Thin films of doped lanthanum manganites like La$_{0.7}$Ca$_{0.3}$MnO$_3$ (LCMO) show a distinctive colossal magneto resistance. In this work we report on x-ray photoelectron diffraction (XPD) measurements of LCMO films (grown by pulsed laser deposition) and of SrTiO$_3$ (STO). The presented polar scans were measured in [100]- and [110]-direction in both cases. In the case of STO the measured polar scans are typical of a cubic crystal structure. In comparison to that the polar scans of LCMO indicate a strained structure.

DS 29.44 Wed 15:00 Poster A

Sb-Bi thin films investigated by structural and optical methods — •Anja König, Peter Zalden, Gunnar Bruns, and Matthias Wuttig — I. Physikalisches Institut (IA), RWTH Aachen, 52056 Aachen, Germany

Phase-change materials (PCMs) offer a significant optical contrast as well as a distinct difference in electronic resistivity between their amorphous and crystalline state. Moreover, they can be rapidly switched between these states thus making them a promising material for non-volatile electronic memories. The crystalline phase of these materials shows a large optical dielectric constant, which is explained in terms of a large dynamic charge, also known as resonant bonding. A map for PCMs has been developed on the basis of a fundamental understanding of the bonding characteristics [1]. However, stoichiometric trends in terms of the dynamic charge and its origin are yet to be investigated.

Therefore, in this study binary Sb-Bi thin films were evaporated in varying stoichiometry and examined structurally (XRD, XRR) and optically (ellipsometry). The binary Sb-Bi system was chosen since these alloys provide three p-electrons per atom throughout, thus fulfilling the prerequisite to be accurately described by the map in every stoichiometry. Additionally, they show a stoichiometric trend regarding

the magnitude of the rhombohedral distortion, which is a well know property of some phase-change materials. These trends can be related to a change in the electronic and structural properties, e.g. a varying magnitude of the rhombohedral distortion.
[1] D. Lencer et al., Nature Materials 7, 972 (2008)

DS 29.45 Wed 15:00 Poster A

Structural and electrical properties of SrTiO3 films grown on CeO2 buffered sapphire — •Eugen Hollmann, Rolf Kutzner, Jurgen Schubert, Gregor Mussler, and Roger Wördenweber — Institute for Bio- and Nanosystems (IBN2), Research Center Juelich, Germany

The physical properties of complex oxides like ferroelectric perovskite are strongly connected with their composition, structure and structural imperfections. Lattice constants and thermal properties of substrate materials and deposited films are usually different. In the case of thin epitaxial films this difference can be used for engineering of properties of ferroelectric materials via mechanical strain due to changing of film thickness and preparation conditions.

In the present work we report on results of measuring the strain of both in buffer CeO2 and STO films on r-cut sapphire. Ferroelectric films were deposited by PLD. Different types of strain lead to various structural modifications in films. The resulting type of distortion and defects are investigated by high-resolution x-ray analysis. Electrical properties of STO films of various thicknesses are measured using planar capacitors in a wide frequencies range.

It is shown that in the thinner films the stress is compensated by misfit dislocations generated during growth and a deformation of the STO lattice. With increasing film thickness cracks develop in two crystalline directions, i.e. along the [1210] and, additionally, the [1010] directions of r-cut sapphire. The strained films show a strong modification of temperature dependence of the dielectric permittivity.

DS 29.46 Wed 15:00 Poster A

Structure analysis of CoFeB/MgO interfaces by focus series reconstruction — •Henning Schuhmann[1], Patrick Peretzki[1], Gerrit Eilers[2], Michael Seibt[1], Markus Münzenberg[2], Volker Drewello[3], Andy Thomas[3], and Günter Reiss[3] — [1]IV. Physikalisches Institut, Georg-August-Universität Göttingen, Germany — [2]I. Physikalisches Institut, Georg-August-Universität Göttingen, Germany — [3]Thin films and Physics of Nanostructures, Universität Bielefeld, Germany

The amorphous CoFeB/ crystalline MgO interface is a fundamental part of magnetic tunnel junctions (MTJ) which are a potential candidate for magnetic random access memory. For these applications a high tunnel magnetoresistance (TMR) is required. Ab initio supercell calculations by Heiliger et al. [1] show, that the TMR increases rapidly with the number of crystalline Fe monolayers at the interface.

These predictions are to be compared with quantitative analysis by high resolution transmission electron microscopy (HRTEM). The cross-section TEM specimens were prepared by Focused Ion Beam (FIB) and conventional techniques.

Using object wave reconstruction from defocus series, local long-range order at these interfaces is investigated. Combined with electrical characterization of TMR devices the correlation of interfacial order and TMR values is investigated.

[1] Ch. Heiliger, M. Gradhand, P. Zahn and I. Mertig, Phys. Rev. Lett. 99, 066804 (2007)

DS 29.47 Wed 15:00 Poster A

Structural optimization of CoFeB/MgO/CoFeB TMR elements — •Patrick Peretzki[1], Vladyslav Zbarskyy[2], Marvin Walter[2], Henning Schuhmann[1], Michael Seibt[1], and Markus Münzenberg[2] — [1]IV. Physikalisches Institut, Georg-August-Universität Göttingen, Germany — [2]I. Physikalisches Institut, Georg-August-Universität Göttingen, Germany

The Tunnel magnetoresistance (TMR) effect is being used in magnetic tunnel junctions (MTJs) consisting of two ferromagnetic electrodes separated by an insulator for a variety of present and future applications. Practical use requires a high junction quality mainly measured in terms of the "TMR value". MTJs are manufactured as a structure of nm scaled layers, a process which can be optimized in many ways to improve the TMR value.

We fabricated MTJs consisting of MgO insulating tunnel barriers and CoFeB ferromagnetic electrodes on MgO substrates. These structures are not suited for practical use, however they show a visible TMR effect under laboratory conditions. Furthermore, they are dedicated to study crystallization processes at MgO/CoFeB interfaces while keeping the manufacturing process simple and easy to control. MgO was grown by Molecular Beam Epitaxy and the CoFeB layers were sputtered in the same chamber. The structures were then analysed by High Resolution Transmission Electron Microscopy for smooth MgO layer growth and crystallization. Various preparation parameters were changed in order to find optimal growth conditions for high TMR values.

We thank the DFG for funding the research through SFB602.

DS 29.48 Wed 15:00 Poster A

Strain, stress and structural analysis of manganite and cobaltate thin films — •Thilo Kramer, Mike Vogt, Stefanie A. Wiedigen, Joerg Hoffmann, and Christian Jooss — Institute of Material Physics, University of Goettingen, Germany

Due to their unusual magnetic and electronic properties complex oxides like Manganites and Cobaltates are promising materials for new functionalities and novel applications. For example, these oxides reveal interesting thermoelectric properties and persistent resistance changes which might be used for energy conversion and data storage. However, these properties are extremely sensitive with respect to crystallographic disorder and strain commonly present in thin films. As model systems we have prepared thin films of $\mathrm{Pr}_{1-x}\mathrm{Ca}_x\mathrm{MnO}_3$ (PCMO) and $\mathrm{Pr}_{1-x}\mathrm{Ca}_x\mathrm{CoO}_3$ by an ion beam sputtering technique. The strain-stress relation with respect to the exact deposition condition is analyzed by combining an in-situ measurement of the substrate bending (Stoney equation) and ex-situ X-ray investigations ($\mathrm{Sin}^2\ \Psi$ -method). This allows to estimate the elasticity modulus and the Poisson ratio of PCMO to about E=94 GPa and ν=0.25. For analysing the early stage of film growth with respect to crystallographic order and surface roughness RHEED measurements are performed during the film growth. Extending both in-situ analytical techniques (stress measurement, RHEED) to high-temperature deposition processes, first results concerning the temperature dependence of stress development and film growth will be presented.

DS 29.49 Wed 15:00 Poster A

Plasma treatment of polydimethylsiloxane thin films — •Vladimir Danilov, Jürgen Meichsner, and Hans-Erich Wagner — Institute of Physics, University of Greifswald, Felix-Hausdorff-Str. 6, 17487 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 (10 nm - 100 nm) were prepared on aluminium coated glass substrates, and their thickness was measured by spectroscopic ellipsometry. The direct plasma treatment is compared with the plasma radiation, only, in argon and hydrogen rf plasmas, respectively. Evolution of IR spectra was monitored, and the changes of PDMS characteristic absorption bands (absorbance, broadening, shifting) as well as the formation of new bands are discussed. In particular, the appearance of new band at 1230 cm^{-1} was observed, and it was identified as LO phonon band of $\mathrm{SiO_x}$. For analysis of the Si-O-Si asymmetrical vibration band the deconvolution of this band was performed using Gaussian peaks.

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Characterization of Plasma Polymerized Ethylenediamine Thin Films for Biomedical Applications — •Frank Wienholtz, Holger Testrich, and Jürgen Meichsner — Institute of Physics, University of Greifswald, Felix-Hausdorff-Str. 6, 17487 Greifswald

Plasma polymerized ethylenediamine (PPEDA) thin films (15 - 80 nm) were deposited on different substrate materials (TiOx, Si, Al) in capacitively coupled radio frequency plasma. Beside the optimization of the plasma processing parameters, the plasma chemical conversion of the precursor ethylenediamine (EDA) was studied by means of the plasma induced optical emission spectroscopy, analysing the CN emission at 384 nm as well as the emission of H_α (656 nm) and Ar (750 nm). The FTIR (IRRAS) absorption spectra of deposited thin films reveal characteristic absorption of NH (3000 and 3500 cm^{-1}), CH (2900 cm^{-1}), CN/CC (2150 cm^{-1}), and NH_2 (1600 cm^{-1}). Comparing the thin film spectra with that of the liquid precursor EDA, the films are strongly cross linked. The refractive index shows normal dispersion in the visible spectral region, and in dependence on the deposition parameters anomal dispersion in the UV. The XPS analysis combined with derivatisation technique provides information about the NH_2 functional groups. Biomedical test substrates covered with PPEDA thin films show significant increase in cell adhesion. The investigations were realized within the BMBF collaborative research project

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Organic molecular beam deposition of organic radicals — •Sabine-A. Savu[1], Indro Biswas[1], Donella Rovai[2], Lorenzo Sorace[2], Matteo Mannini[2], Andrea Caneschi[2], Antje Vollmer[3], M. Benedetta Casu[1], and Thomas Chassé[1] — [1]IPTC, University of Tübingen, Tübingen, Germany — [2]LAMM, University of Florence, Italy — [3]Helmholtz-Zentrum Berlin, BESSY, Berlin, Germany

Nitronyl nitroxide radicals are a class of paramagnetic compounds that are of interest not only because of their magnetic properties but also because of their use as a building block in more complex magnetic structures. A crucial aspect is the possibility to grow thin films, down to the submonolayer regime, investigating their chemical, physical, and morphological properties. In this work we present X-ray photoelectron spectroscopy (XPS), atomic force microscopy (AFM), and NEXAFS (Near Edge X-ray Absorption Fine Structure), of thin films of a pyrene derivative of the nitronyl nitroxide radical (nitpyrene). Nitpyrene was deposited under ultra high vacuum conditions onto the well characterized single crystal Au(111) surface, using strictly controlled evaporation conditions. The electronic structure and the interaction with the surface are discussed. By analyzing the attenuation of the XPS substrate signal, we find indications for a Stranski-Krastanov growth mode, supported by AFM measurements showing a distinctive island formation under this preparation conditions. The persistence of the paramagnetic character of the molecules has been probed by EPR measurements.

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Investigation of the chemical and electronic structure of CoPc from sub-monolayer to thick films by photoemission spectroscopy — •Uwe Treske, Feng Zhu, Mandy Grobosch, and Martin Knupfer — IFW Dresden

We have grown highly oriented films of cobalt(II) phthalocyanine (CoPc) under ultra high vacuum conditions on single crystalline Au(001)-5x20 surfaces. The molecular orientation and ordering have been studied by low energy electron diffraction (LEED). LEED patterns taken for sub-monolayer up to several nm thick CoPc films reveal highly ordered CoPc films. Within the films the molecules lie with their molecular axis parallel to the Au(001)-5x20 surface. By means of combined X-ray and ultraviolet photoemission spectroscopy (XPS, UPS) we have investigated the chemical and electronic structure of the CoPc films for all thicknesses. Our results indicate a clear difference in the valence band spectra for sub-monolayer and several nm thick CoPc films due to a possible influence of image charge screening effects on the molecular orbitals in the vicinity of the Fermi level.

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Anomalous hysteresis loops measured by magneto-optical Kerr effect in Ni/rubrene bilayers — •Wen Li[1], Michael Fronk[1], Felix Springer[2], Hartmut Kupfer[1], Steffen Schulze[1], Michael Hietschold[1], Manfred Albrecht[1], Dietrich R. T. Zahn[1], and Georgeta Salvan[1] — [1]Institute of Physics, Chemnitz University of Technology, D-09107 Chemnitz, Germany — [2]Department of Physics, University of Konstanz, D-78457 Konstanz, Germany

Metal/organic heterostructures formed by the deposition of metals on organic films find a wide application range in organic electronics and spintronics. In this work Ni(14 nm)/rubrene(15 nm) bilayers were fabricated by subsequent deposition in ultra-high vacuum. For the very low evaporation rate used for the rubrene deposition, the bilayer morphology is characterized by large, well separated islands. The magnetic and structural properties of the heterostructure were probed by SQUID, AFM and TEM measurements, respectively. The magneto-optical Kerr effect (MOKE) of this ferromagnetic/organic bilayer was measured in the energy range from 1.5 eV to 5.5 eV. At photon energies near the zero crossing point in the real part of the MOKE spectrum, anomalous hysteresis shapes were obtained. The numerical analysis of the MOKE hysteresis at several photon energies reveals the combination of two components with orthogonal magnetization or different anisotropy.

DS 29.54 Wed 15:00 Poster A

Identifikation of molecular orbitals of FePc near the chemical potential. — •Friedrich Roth, Andreas König, Roberto Kraus, Mandy Grobosch, Thomas Kroll, Martin Knupfer, and Bernd Büchner — IFW Dresden, P.O. Box 270116, D-01171 Dresden, Germany

We have studied the electronic structure of iron phthalocyanine (FePc) films at low temperature using electron energy-loss spectroscopy. The electronic excitation spectrum of FePc is rather complex and comprises both π-π^* transitions of the phthalocyanine ligand and transitions that involve the Fe 3d orbitals. The C1s core excitations provide so far unidentified information on the molecular orbitals. They demonstrate that the Fe 3d orbital with e_g symmetry lies energetically in between the highest occupied and the lowest unoccupied ligand state and that it is not fully occupied.

DS 29.55 Wed 15:00 Poster A

Electronic excitations of potassium doped MnPc — •Benjamin Mahns, Friedrich Roth, Andreas König, Roberto Kraus, Mandy Grobosch, Sven Partzsch, Martin Knupfer, and Bernd Büchner — IFW Dresden, P.O. Box 270116, D-01171 Dresden, Germany

We have investigated the evolution of the electronic excitations of Manganese Phthalocyanine (MnPc), an archetype magnetic molecule, upon potassium doping using Electron Energy-Loss Spectroscopy. Thin films of MnPc have been grown by thermal evaporation on orientated KBr (100) crystals under Ultra High Vacuum conditions. A characterization of the crystal structure using electron diffraction and optical spectroscopy shows that we are mainly dealing with the so called α-polymorph of MnPc. We also could identify stable phases of K_2MnPc and K_4MnPc. Potassium doping, i.e. the addition of electrons to the MnPc molecules, causes significant changes in the electronic excitations involving π-π^* transitions of the pthalocyanine ligand as well as the Mn 3d orbitals.

DS 29.56 Wed 15:00 Poster A

Determination of the spin and orbital ground state of transition metal phthalocyanines — •Thomas Kroll[1], Roberto Kraus[1], Mandy Grobosch[1], Olga V. Molodtsova[1], Victor Yu. Aristov[1,2], Patrick Hoffmann[3], and Martin Knupfer[1] — [1]IFW Dresden, P.O. Box 270016, D-01171 Dresden, Germany — [2]Institute of Solid State Physics, Russian Academy of Sciences, Chernogolovka, Moscow distr. 142432, Russia — [3]Helmholtz-Zentrum Berlin für Materialien und Energie, Bessy II, Berlin, Germany

The electronic structure of magnetic molecular materials such as metal phthalocyanines (MPc) systems has been investigated by means of soft X-ray absorption, photoemission and resonant photoemission spectroscopy.

In these systems, a transition metal ion is incorpaorated into the center of a phthalocyanine complex, that determines all magnetic properties of the molecule. Even though various suggestions on the ground state structure of these MPc's have been proposed, no satisfactory picture could be derived, yet. Only the corresponding spin is well known, including the unusual intermediate spin state for FePc and MnPc. With the help of these spectroscopic methods for different polarisation and temperatures, we shed a brighter light on the electronic structure of various MPc's and, together with theoretical calculations, clarify the exact structure of their ground and excited states.