Thin Films Division
Fachverband Dünne Schichten (DS)

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Overview of Invited Talks and Sessions

(Lecture Rooms H3, H8, and H32; Poster B1 and B2)

Plenary, Keynote and Prize Talks related to Division DS

DS 22.1	Wed	13:15–13:55	H15	**Complex magnetic order on the atomic scale** — •Kirsten von Bergmann
DS 33.1	Fri	8:30– 9:15	H1	**Templated Self-assembly of Block Copolymer Films** — •Caroline Ross

Tutorial Integration and Modelling of Nanoelectronic Components

DS 1.1	Sun	16:00–16:30	H3	**Current transport through nanoscale electronic components** — •Artur Erbe
DS 1.2	Sun	16:35–17:05	H3	**Theory of electronic transport in single-molecule junctions** — •Juan Carlos Cuevas
DS 1.3	Sun	17:10–17:40	H3	**DNA-programmed assembly of dendrimers and conjugated polymers** — •Kurt Gothelf
DS 1.4	Sun	17:45–18:15	H3	**Silicon Nanowires: A Versatile Technology Platform for Nanoelectronic Research** — •Thomas Mikolajick, Andre Heinzig, Jens Trommer, Dominik Martin, Matthias Grube, Andreas Krause, Walter Weber

Invited and Topical Talks

DS 2.1	Mon	9:30–10:00	H32	**Mechanisms of ion beam induced surface pattern formation** — •Thomas Michely
DS 2.2	Mon	10:00–10:30	H32	**Mechanisms of surface pattern formation under irradiation with heavy ions** — •Karl-Heinz Heinig, Bartosz Liedke, Herbert Urbassek, Christian Anders, Lothar Bischoff, Roman Böttger
DS 2.3	Mon	10:30–11:00	H32	**Interaction of energetic ultraheavy ions with surfaces** — •Lothar Bischoff, Roman Böttger, Karl-Heinz Heinig
DS 2.4	Mon	11:15–11:45	H32	**Quantitative analysis of nanoripple patterns by GISAXS 3D mapping** — •David Babonneau, Elliot Vandenhecke, Mathieu Garel, Sophie Camelio, Sophie Rousselet
DS 2.5	Mon	11:45–12:15	H32	**Movement of a ripple pattern by ion beam irradiation** — •Paul Alkemade
DS 2.6	Mon	12:15–12:45	H32	**Redeposition during ion-beam erosion** — Nils Anspach, Christian Diddens, Marc Osthues, •Stefan Linz
DS 14.1	Tue	9:30–10:00	H8	**Nanowire photovoltaics with absorption beyond the ray optics limit.** — •Magnus T Borgström
DS 14.2	Tue	10:00–10:30	H8	**Crystal structure control in nanowires** — •Erik Bakkers
DS 14.3	Tue	10:30–11:00	H8	**Spectral and spatial overlap of oxide quantum wells and whispering gallery modes** — •Marius Grundmann

DS 14.4	Tue	11:15–11:45	H8	**Semiconducting Nanowire Heterostructures on Silicon - From Growth to Devices** — Heinz Schmid, Kirsten Moselund, Cedric Bessire, Pratyush Das Kanungo, Philipp Mensch, Siegfried Karg, Mattias Borg, Volker Schmidt, •Heike Riel
DS 14.5	Tue	11:45–12:15	H8	**III-nitride nanowires: From growth phenomena to light-emitting diodes** — •Raffaella Calarco
DS 14.6	Tue	12:15–12:45	H8	**3D GaN nanorods: fabrication, properties, applications** — •Andreas Waag, Johannes Ledig, Xue Wang, Milena Erenburg, Jana Hartmann, Lorenzo Caccamo, Matin Mohajerani, Manal Ali Deeb, Jiandong Wei, Martin Hoffmann, Hao Shen, Hergo-Heinrich Wehmann
DS 17.1	Wed	9:30–10:00	H32	**Meso-Superstructured Perovskite Solar Cells** — •Henry J. Snaith
DS 17.2	Wed	10:00–10:30	H32	**Thermoelectric perovskite-type oxides and Heusler phases** — •Anke Weidenkaff, Sascha Populoh, Leyre Sagarna, Gesine Saucke, Andrey Shkabko, Nina Vogel
DS 17.3	Wed	10:30–11:00	H32	**Photoelectrochemical Water Splitting with Complex Metal Oxides: the Role of Defects** — •Roel van de Krol
DS 17.4	Wed	11:15–11:45	H32	**Intrinsic point defects in $CuInSe_2$ and $CuGaSe_2$ studied by screened-exchange hybrid density functional theory** — •Karsten Albe, Johan Pohl
DS 17.5	Wed	11:45–12:15	H32	**Energy Band Alignment in Thin Film Solar Cells** — •Andreas Klein
DS 17.6	Wed	12:15–12:45	H32	**Nanowire device concepts for thin film photovoltaics** — •Silke Christiansen
DS 29.1	Thu	9:30–10:00	H32	**Organic Magnetoresistance: The effect of excitons on charge transport in organic semiconductors** — •William Gillin
DS 29.2	Thu	10:00–10:30	H32	**Metal-phthalocyanines: Materials for molecular spintronics** — •Jens Kortus, Rico Friedrich, Torsten Hahn, Claudia Loose, Martin Knupfer
DS 29.3	Thu	10:30–11:00	H32	**Magneto-optical Kerr Effect Spectroscopy of Selected Phthalocyanines and Porphyrines** — •Georgeta Salvan, Peter Robaschick, Frank Lungwitz, Michael Fronk, Carola Mende, Heinrich Lang, Rico Friedrich, Jens Kortus, Dietrich R.T. Zahn
DS 29.4	Thu	11:00–11:30	H32	**Molecular Quantum Spintronics** — •Mario Ruben
DS 29.5	Thu	11:45–12:15	H32	**Nanomembrane based electrodes for contacting ultra-thin organic layers** — •Carlos Cesar Bof Bufon, Celine Vervacke, Maria Esperança Navarro Fuente, Dominic J. Thurmer, Christian Müller, Michael Fronk, Georgeta Salvan, Dietrich R. T. Zahn, Oliver G. Schmidt
DS 29.6	Thu	12:15–12:45	H32	**Spinterfaces as microscopic spin traps** — •Mirko Cinchetti

Invited talks of the joint symposium SYCT

See SYCT for the full program of the symposium.

SYCT 1.1	Mon	9:30–10:00	H1	**A coarse grained QM/MM approach for the description of charge transfer in complex systems** — •Marcus Elstner
SYCT 1.2	Mon	10:00–10:30	H1	**Identifying and resolving charge separation in organic solar cells** — •Eberhard Riedle
SYCT 1.3	Mon	10:30–11:00	H1	**Quantifying the energy of charge transfer states: From molecular crystals to donor-acceptor blends** — •Reinhard Scholz
SYCT 1.4	Mon	11:00–11:30	H1	**Efficient Exciton Generation and Collection in Organic Solar Cells** — •Mark Thompson, Cong Trinh, Steve Forrest, Jeramy Zimmerman
SYCT 1.5	Mon	11:30–12:00	H1	**Electron transport in organic single-crystal transistors and Schottky-gated heterostructures** — •Alberto Morpurgo

Invited talks of the joint symposium SYTS

See SYTS for the full program of the symposium.

SYTS 1.1	Wed	9:30–10:00	H1	**Transport in Old and New Thermoelectric Materials** — •David Singh
SYTS 1.2	Wed	10:00–10:30	H1	**Binary oxide structures as model systems for thermoelectric transport** — •Peter J. Klar, Christian Heiliger
SYTS 1.3	Wed	10:30–11:00	H1	**Functional oxides films: from single crystals to polycrystalline substrates** — •Wilfrid Prellier

SYTS 1.4	Wed	11:00–11:30	H1	**The Planar Nernst Effect and the Search for Thermal Spin Currents in Ferromagnetic Metals** — •Barry Zink
SYTS 1.5	Wed	11:30–12:00	H1	**Tunneling magneto thermopower in magnetic tunnel junction nanopillars** — Niklas Liebing, Santiago Serrano-Guisan, Patryk Krzysteczko, Karsten Rott, Günter Reiss, Jürgen Langer, Berthold Ocker, •Hans Werner Schumacher

Invited talks of the joint symposium SYES

See SYES for the full program of the symposium.

SYES 1.1	Fri	9:30–10:00	H1	**Molecular dynamics simulation of nucleation and growth of crystals from solution** — •Michele Parrinello
SYES 1.2	Fri	10:00–10:30	H1	**Describing, understanding, and discovering hybrid materials from first principles** — •Claudia Draxl
SYES 1.3	Fri	10:30–11:00	H1	**Mapping the Electronic Structure Landscape for Materials Discovery** — •Krishna Rajan
SYES 1.4	Fri	11:00–11:30	H1	**New ferroelectrics and antiferroelectrics by design** — •Karin Rabe
SYES 1.5	Fri	11:30–12:00	H1	**The Materials Project: The design of materials using high-throughput ab initio computations** — •Gerbrand Ceder

Sessions

DS 1.1–1.4	Sun	16:00–18:15	H3	**Tutorial: Integration and Modelling of Nanoelectronic Components**
DS 2.1–2.6	Mon	9:30–12:45	H32	**Focus Session: Ion Beam Induced Surface Patterns I**
DS 3.1–3.10	Mon	9:30–12:00	H3	**Multiferroics 1 (jointly with DF, KR, MA, TT)**
DS 4.1–4.3	Mon	12:15–13:00	H8	**Atomic Layer Deposition**
DS 5.1–5.5	Mon	12:15–13:30	H1	**Charge Transfer Effects in Molecular Materials I (jointly with BP, CPP, HL)**
DS 6.1–6.5	Mon	14:45–16:00	H8	**Focus Session: Ion Beam Induced Surface Patterns II**
DS 7.1–7.13	Mon	15:00–18:30	H3	**Multiferroics 2 (jointly with DF, KR, MA, TT)**
DS 8.1–8.7	Mon	15:00–17:30	H40	**Charge Transfer Effects in Molecular Materials II (jointly with BP, CPP, HL)**
DS 9.1–9.4	Mon	16:15–17:15	H8	**Ion and Electron Beam Induced Processes**
DS 10.1–10.6	Mon	17:15–18:45	H32	**Organic Electronics and Photovoltaics I (jointly with CPP, HL, O)**
DS 11.1–11.23	Mon	17:00–20:00	Poster B1	**Poster Session I: Application of thin films; Ion beam induced surface patterns; Ion and electron beam induced processes; Micro- and nanopatterning (jointly with O)**
DS 12.1–12.24	Mon	17:00–20:00	Poster B1	**Poster Session II: Functionalized semiconductor nanowires (jointly with HL); Resistive switching (jointly with DF, KR, HL); Thermoelectric materials**
DS 13.1–13.22	Mon	17:00–20:00	Poster B1	**Poster Session III: Layer properties: electrical, optical and mechanical properties; Thin film characterization: structure analysis and composition (XRD, TEM; XPS, SIMS, RBS..)**
DS 14.1–14.6	Tue	9:30–12:45	H8	**Focus Session: Functionalized Semiconductor Nanowires I (jointly with HL)**
DS 15.1–15.12	Tue	9:30–12:45	H32	**Organic Electronics and Photovoltaics II (jointly with CPP, HL, O)**
DS 16.1–16.6	Tue	14:45–16:15	H32	**Organic Thin Films I**
DS 17.1–17.6	Wed	9:30–12:45	H32	**Focus Session: Thin Film Photovoltaic Materials and Solar Cells I**
DS 18.1–18.8	Wed	9:30–11:30	H8	**Micro- and Nanopatterning (jointly with O)**
DS 19.1–19.10	Wed	9:30–12:15	H23	**Spin Effects in Molecules at Surfaces (jointly with MA, O)**
DS 20.1–20.3	Wed	9:30–10:30	H11	**High- and Low-k-Dielektrics (jointly with DF)**
DS 21.1–21.4	Wed	11:45–12:45	H8	**Focus Session: Functionalized Semiconductor Nanowires II (jointly with HL)**
DS 22.1–22.1	Wed	13:15–13:55	H15	**Gaede Prize Talk - Kirsten von Bergmann**
DS 23.1–23.13	Wed	14:45–18:15	H8	**Focus Session: Thin Film Photovoltaic Materials and Solar Cells II**

DS 24.1–24.9	Wed	14:45–17:00	H32	**Thermoelectric Materials**
DS 25.1–25.5	Wed	15:00–17:30	H10	**Focus Session: Magnetic Damping Phenomena in Thin Films and Nanostructures (jointly with MA)**
DS 26.1–26.12	Wed	16:00–19:00	H33	**Organic Electronics and Photovoltaics (jointly with CPP, HL, O)**
DS 27.1–27.10	Wed	17:15–19:45	H32	**Thin Film Characterization: Structure Analysis and Composition (XRD, TEM, XPS, SIMS, RBS,...) I**
DS 28.1–28.13	Thu	9:30–13:00	H8	**Layer Properties: Electrical, Optical, and Mechanical Properties**
DS 29.1–29.9	Thu	9:30–13:30	H32	**Focus Session: Organic Materials for Spintronics: From Spinterface to Devices (jointly with HL, MA, O)**
DS 30.1–30.10	Thu	14:45–17:15	H32	**Thin Film Characterization: Structure Analysis and Composition (XRD, TEM, XPS, SIMS, RBS,...) II**
DS 31.1–31.9	Thu	14:45–17:00	H8	**Organic thin films II**
DS 32.1–32.62	Thu	17:00–20:00	Poster B2	**Poster Session IV: Atomic layer deposition; Organic thin films; Organic Electronics and Photototovoltaics; Organic Materials for Spintronics - from spinterface to devices; Thin film photovoltaic materials and solar cells**
DS 33.1–33.1	Fri	8:30– 9:15	H1	**Plenary Talk - Caroline Ross**
DS 34.1–34.12	Fri	9:30–12:45	H32	**Resistive Switching (jointly with DF, KR, HL)**
DS 35.1–35.10	Fri	9:30–12:00	H8	**Application of Thin Films**

Annual General Meeting of the Thin Films Division

Monday 19:00–20:00 Room H32

Mitgliederversammlung der Deutschen Vakuumgesellschaft e.V. (DVG)

Monday 18:15–19:00 M 102

DS 1: Tutorial: Integration and Modelling of Nanoelectronic Components

The development of novel nanoelectronic components, e.g. semiconductor nanowires, single organic molecules or magnetic nanoparticles, aims at the creation of electronic circuits at the smallest possible length scale. A first prerequisite for the construction of such electronic components is the formation of a reliable, electrical contact to the electrically active parts and their integration into larger networks. This can be achieved either by self organization or by novel lithography methods. Reliable circuits can only be built if effects arising from transport through individual nanostructures as well as collective effects caused by the integration of the nanostructures into larger networks are well understood and controlled. This tutorial will provide an overview on the experimental realization of the contacts, modeling of the systems, and possible schemes for the development of larger circuits. The introductory talks in this tutorial will be presented by members and collaborators of the International Helmholtz Research School NanoNet, which deals with the development of nanoelectronic circuits.(Organizer: Artur Erbe, Helmholtz-Zentrum Dresden-Rossendorf)

Time: Sunday 16:00–18:15 Location: H3

Tutorial DS 1.1 Sun 16:00 H3

Current transport through nanoscale electronic components — •Artur Erbe — Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany

The semiconductor industry has been scaling down electronics in the course of the past decades. It is clear that at the current speed of miniaturization fundamental limits will restrict the further development of nanoelectronics. Therefore, alternative ways for building electronics need to be developed. Possible candidates for active nanoelectronic building blocks are single organic molecules or metallic nanoparticles. The first step in building electronic circuits from these single components is the definition of a reliable contact to external connections. In this talk an overview on contacting schemes will be given and their advantages and problems will be discussed. Typical results, which have been found on single molecules and metallic nanoparticles using these techniques, will be presented. These facts clearly show that nanoelectronic components for future electronic are already being developed and that the next step in these developments will be the interconnecting of these single building blocks in order to produce integrated circuits.

Discussion (5 min)

Tutorial DS 1.2 Sun 16:35 H3

Theory of electronic transport in single-molecule junctions — •Juan Carlos Cuevas — Departamento de Fisica Teorica de la Materia Condensada, Universidad Autonoma de Madrid, E-28049 Madrid (Spain)

The recent advancements in nanofabrication techniques have allowed to contact individual molecules between metallic electrodes and to investigate their transport properties. This has posed a formidable challenge for the theory, namely to elucidate the physical mechanisms that dominate the electronic conduction at the nanoscale. In this talk I will briefly review some of the theoretical techniques and tools that are currently being used to describe the transport properties of single-molecule junctions, and I will discuss the novel transport phenomena that occur in these systems.

Discussion (5 min)

Tutorial DS 1.3 Sun 17:10 H3

DNA-programmed assembly of dendrimers and conjugated polymers — •Kurt Gothelf — Aarhus University, Aarhus, Denmark

The idea behind our research is to use DNA as a programmable tool for directing the self-assembly of molecules and materials. The unique specificity of DNA interactions, our ability to code specific DNA sequences and to chemically functionalize DNA, makes it the ideal material for controlling self-assembly of components attached to DNA sequences. We have developed some new approaches in this area such as the use of DNA for self-assembly of organic molecules[1] and position dendrimers. We have used DNA origami to assemble organic molecules, study chemical reactions with single molecule resolution [4]. We have also formed 3D DNA origami structures [5] and dynamic DNA structures [6]. In the presentation I will focus on our recent progress on self-assembly of macromolecular DNA conjugates such as dendrimers and conjugated polymers into DNA origami.

References [1] Ravnsbaek; J. B et al. Angew. Chem. Int. Ed. 2011, 50, 10851-10854. [3] Liu, H. et al. J. Am. Chem. Soc. 2010, 132, 18054-18056. [4] Voigt, N. V. et al. Nature Nanotech. 2010, 5, 200-205. [5] Andersen, E. S. et al. Nature 2009, 459, 73-76. [6] Zhang, Z. et al. Angew. Chem. Int. Ed. 2011, 50, 3983-3987.

Discussion (5 min)

Tutorial DS 1.4 Sun 17:45 H3

Silicon Nanowires: A Versatile Technology Platform for Nanoelectronic Research — •Thomas Mikolajick[1,2], Andre Heinzig[2], Jens Trommer[1], Dominik Martin[1], Matthias Grube[1], Andreas Krause[1], and Walter Weber[1] — [1]NaMLab GmbH, Nötnitzer Strasse 64, 01187 Dresden — [2]Chair for Nanoelectronic Materials, TU Dresden, Nötnitzer Strasse 64, 01187 Dresden

Silicon nanowire based metal insulator silicon (MIS) devices offer the best gate control and therefore will enable the ultimate scaling of CMOS devices. Moreover, the specific features of a very precise controlled structure and the quasi 1-dimensional geometry (transport) make silicon nanowires an ideal platform for new device concepts like junctionless devices or tunnel field effect transistors. Recently, the reconfigurable field effect transistor (RFET) [1] using the unique properties of silicon nanowires [2] enables the electrical configuration of n- or p-type behavior. In this talk the technology as well as the device properties of the RFET will be explained. It will be shown that the same basic structure can successfully be applied to realize chemical and biochemical sensors. Finally, additional examples of the application of the base technology in anodes for Li-ion batteries will be given. [1] A. Heinzig, et al. Nano Lett. 12, 119 (2012) [2] D. Martin et al. Phys. Rev. Lett. 107, 216807 (2011)

DS 2: Focus Session: Ion Beam Induced Surface Patterns I

Low energy ion irradiation of surfaces is known to induce self-organized nanoscale surface dot or ripple patterns. During the last years several novel experimental and theoretical advances have been accomplished, contributing to a better understanding of the pattern formation mechanisms and allowing fabrication of tailored patterns or very smooth surfaces. Several possible applications of self-organized nanopatterned surfaces for optical and magnetic devices were presented. A variety of systematic experimental data is now available, allowing a profound test of recent theoretical models for pattern formation. This focus session will highlight the recent developments in self-organized pattern formation and new analysis techniques to determine in particular the dynamic behavior of ion-induced surface patterns. (Organizer: Hans Hofsäss, University Göttingen)

Time: Monday 9:30–12:45 Location: H32

Topical Talk DS 2.1 Mon 9:30 H32

Mechanisms of ion beam induced surface pattern formation — •Thomas Michely — II. Physikalisches Institut, Universität zu Köln, Zülpicher Str. 77, 50937 Köln

Related to three different material classes - metals, elemental semiconductors and epitaxial graphene - three different pattern formation mechanisms will be presented. At sufficiently high temperatures ion induced pattern formation on metals may be considered as the inverse of homepitaxial growth and is determined by anisotropies of diffusion related to the crystalline structure. Elemental semiconductors like Si and Ge amorphize under the ion beam at ambient conditions and form patterns most readily in the presence of silicide forming impurities. Finally, ion beam induced pattern formation in epitaxial graphene can originate from an inhomogeneous interaction of graphene with its substrate, driving vacancies into an ordered array of vacancy clusters.

Topical Talk DS 2.2 Mon 10:00 H32

Mechanisms of surface pattern formation under irradiation with heavy ions — •Karl-Heinz Heinig[1], Bartosz Liedke[1], Herbert Urbassek[2], Christian Anders[2], Lothar Bischoff[1], and Roman Böttger[1,3] — [1]Helmholtz-Zentrum Dresden-Rossendorf, POB 51 01 19, 01314 Dresden — [2]Physics Department and Research Center OPTIMAS, University Kaiserslautern, Erwin-Schrödinger-Straße, 67663 Kaiserslautern — [3]Technische Universität Dresden, 01062 Dresden

The driving force for surface pattern formation under ion irradiation has been under discussion for many years. Bradley and Harper suggested that curvature dependent sputtering is the source for the surface instability. Later on, Carter and Vishnyakov concluded that the transfer of the ion momentum to atoms causes a mass drift which smoothes the surface but destabilizes it at large off-normal impact angles. Thus, no pattern formation is expected for normal incidence on elemental semiconductors. However, very recently we found that normal incidence irradiation of Ge with ultraheavy ions (Bi_3^{++} , Bi_2^{+}, 10...20 keV/atom) leads to very pronounced, hexagonally ordered dot pattern [1]. This pattern form if the energy density deposited close to the surface in a single ion impact exceeds a threshold, which can be achieved by ultraheavy ions or by substrate heating [2]. A model of pattern formation based on transient melt pool formation with local surface minimization will be presented. [1] L. Bischoff, K.-H. Heinig, B. Schmidt, S. Facsko, W. Pilz, NIMB 272 (2012) 198; [2] R. Böttger, L. Bischoff, K.-H. Heinig, W. Pilz, B. Schmidt, JVST B30 (2012) 06FF12.

Topical Talk DS 2.3 Mon 10:30 H32

Interaction of energetic ultraheavy ions with surfaces — •Lothar Bischoff, Roman Böttger, and Karl-Heinz Heinig — Helmholtz-Zentrum Dresden-Rossendorf, Germany

Energetic ultraheavy polyatomic ions like Bi_3^{++} and Bi_2^{+} produce very dense collision cascades in surface layers. Compared to monatomic ion impacts, which do not overlap in space and time within the heat relaxation time, the simultaneous impact of a few atoms in the same point can cause very different effects. Here, we report on FIB irradiation with fluences up to 10^{17} cm^{-2} using a liquid metal ion source. Using ultraheavy ions, a significantly increased sputter yield of Ge has been found, which can be attributed to thermal processes. Another, more striking feature is the dramatic difference in the surface morphologies caused by monatomic and ultraheavy ion irradiation. For instance, the well-known spongy surface layer forms on Ge upon 20 keV Bi^+ irradiation, whereas normal incidence Bi_3^{++} irradiation with the same energy per atom results in hexagonally ordered dot pattern having an aspect ratio of about one. Similar pattern have been found on Si by ultraheavy ion irradiation, but only under substantial substrate heating. And, in hot Ge substrates, normal incidence monatomic Bi^+ ions produce no longer Ge sponge but also dot pattern. A crude thermal analysis of the experiments shows that the considered dot pattern formation is associated with a critical energy density deposited by an ion close to the surface. A more comprehensive model on this pattern formation will be presented in a subsequent talk by K.-H. Heinig.
R. Böttger, L. Bischoff, K.-H. Heinig, et al. JVST B30 (2012)06FF12

Coffee break (15 min)

Invited Talk DS 2.4 Mon 11:15 H32

Quantitative analysis of nanoripple patterns by GISAXS 3D mapping — •David Babonneau, Elliot Vandenhecke, Mathieu Garel, Sophie Camelio, and Sophie Rousselet — Institut Pprime, CNRS, Poitiers, France

3D reciprocal space mapping in the grazing incidence small-angle x-ray scattering (GISAXS) geometry was used to obtain accurate morphological characteristics of nanoripple patterns prepared by low energy (500-1500 eV) Xe^+ ion sputtering of Al_2O_3 and Si_3N_4 amorphous thin films at oblique incidence. We will show that appropriate modeling in the distorted wave-Born approximation makes it possible to determine unambiguously the average 3D shape of the ripples (width, height, length, and asymmetry) along with the degree of ordering of the pattern, which strongly depend on the experimental conditions of sputtering such as ion energy, angle of incidence, temperature, ion flux, and total fluence. In addition, we will show that the lateral order of the nanoripple patterns can be transferred to arrays of noble metal nanoparticles (Ag or Au) or magnetic nanowires (FePt) by subsequent ion-beam sputtering deposition at glancing incidence. GISAXS experiments clearly demonstrate that (i) the rippled surfaces are selectively decorated by the nanoparticles/nanowires on the facets that face the incoming atomic flux, and (ii) the growth of an additional capping layer proceeds conformal with respect to the modulation of the prepatterned buffer layer.

Invited Talk DS 2.5 Mon 11:45 H32

Movement of a ripple pattern by ion beam irradiation — •Paul Alkemade — Kavli Institute of Nanoscience, Delft University of Technology, Delft, The Netherlands

When a beam of energetic ions bombards a material, atoms are being sputtered from the material's surface. Even if the surface is initially smooth, the bombardment might induce surface roughness, often in a more or less regular pattern. These patterns can be a nuisance in sputter deposition or 3-dimensional materials analysis, but are also potentially beneficial, e.g. as anti-reflection layers.

Depending on the material's bulk and surface composition, the temperature, and the type, energy and angle of the ion beam different pattern types might evolve. A very common one is a ripple pattern, evolving under off-normal incidence on amorphous surfaces.

Various physical mechanisms can determine the pattern evolution. So far almost all experimental and theoretical studies address the growth or decay of the ripple amplitude. However, study of the lateral movement of the ripples can reveal crucial details of the mechanisms.

The angular dependence of the sputter rate predicts that at off-normal incidence ripples move against the ion beam direction, but recent experiments show otherwise. In this talk I will show that beam-driven viscous flow and relaxation of beam-induced stress can explain the observed direction of the moving ripples.

Topical Talk DS 2.6 Mon 12:15 H32

Redeposition during ion-beam erosion — Nils Anspach, Christian Diddens, Marc Osthues, and •Stefan Linz — Institut für Theoretische Physik, WWU Münster

Redeposition, i.e. the effect that eroded target particles generated by ion-beam erosion processes can, at least partially, attach to the target surface again, has been scarcely studied in the past. This inherently non-local effect can have substantial impact on the nano-scale evolution of the surface morphology of the eroded target. Using an appropriately tailored one-dimensional solid-on-solid model [1] and a two-dimensional continuum formulation [2] for redeposition processes, we investigate their generic physical properties on the nanoscale. Most significantly, by combining the redeposition model with standard models for erosion, we are able to verify that redeposition can potentially stabilize well-ordered hexagonal nanostructures, as also detected in low-energy ion-beam erosion experiments on semiconductors.

[1] N Anspach, S Linz, J. Stat. Mech. 2012, P06012; 2010, P06023
[2] C Diddens, S Linz, in preparation

DS 3: Multiferroics 1 (jointly with DF, KR, MA, TT)

Time: Monday 9:30–12:00 Location: H3

DS 3.1 Mon 9:30 H3

Magnetoelectric coupling at the *n*-doped interface BaTiO$_3$/SrTcO$_3$ studied from first principles — •Vladislav Borisov[1], Sergey Ostanin[1], and Ingrid Mertig[1,2] — [1]Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle, Germany — [2]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, D-06099 Halle, Germany

Antiferromagnetically induced magnetoelectric coupling at the interface BaTiO$_3$/SrTcO$_3$, which combines a robust ferroelectric and a stable antiferromagnetic perovskite, is studied from first principles. For the BaO/TcO$_2$-terminated interface, the magnetic order may change from G- to C-type antiferromagnetism upon the electric polarization reversal in the ferroelectric side. By inspecting the two-dimensional band structure and orbital occupation of the Tc 4*d*-states we conclude that the polarization-dependent charge transfer is responsible for a two-dimensional electron gas at the interface between two insulating perovskites. The case of paraelectric BaTiO$_3$ is also discussed in the context of the effect.

DS 3.2 Mon 9:45 H3

Observation of novel multiferroic-like effect in C60-Co nanocomposites — •Masashi Shiraishi[1], Eiiti Tamura[1], Yutaka Sakai[1], Toyokawa Shuhei[1], Eiji Shikoh[1], Vlado Lazarov[2], Atsufumi Hirohata[3], Teruya Shinjo[1], and Yoshishige Suzuki[1] — [1]Graduate School of Engineering Science, Osaka Univ., Japan — [2]Department of Physics, Univ. York, UK — [3]Department of Electronics, Univ. York, UK

A novel magnetoelectric effect is found to appear in a C60-Co nanocomposite. Although Co is well-known as a ferromagnet, its nanoparticles embedded in a C60 matrix can exhibit enhancement of magnetoresistance ratio due to a combination of Coulomb-blockade and higher order co-tunneling [1], and also multiferroic-like behavior [2], i.e., an electric field controls magnetic alignment of the nanoparticles and a magnetic field controls their charged states. This novel effect enables a strong magnetic switching effect for which the on/off ratio is ca. 1e4. Such an effect has been expected to exist and these findings show this magnetoelectric coupling for the first time.

[1] D. Hanataka, M. Shiraishi et al., Phys. Rev. B79, 235402 (2009). [2] Y. Sakai, E. Tamura, M. Shiraishi et al., Adv. Func. Mat. 22, 3845 (2012).

DS 3.3 Mon 10:00 H3

Investigation of magnetic ordering in Eu$_{1-x}$Y$_x$MnO$_3$ using full polarization analysis at P09 beamline — •Arvid Skaugen, Dinesh K. Shukla, Helen Walker, Sonia Francoual, and Jörg Strempfer — Deutsches Elektronen-Synchrotron, Harmburg, Germany

Varying multiferroic properties with strong ME coupling have been reported for Eu$_{1-x}$Y$_x$MnO$_3$ [1]. The crystal structure of Eu$_{1-x}$Y$_x$MnO$_3$ is similar to the one of TbMnO$_3$ with comparable lattice distortions. However, the effect of rare earth magnetism is eliminated since Eu^{3+} (4f^6) and Y^{3+} (4f^0) ions both are non-magnetic. The compound Eu$_{0.8}$Y$_{0.2}$MnO$_3$ first shows a phase transition at T$_N$ = 45K from a paramagnetic to an antiferromagnetic and paraelectric state with a presumably sinusoidal collinear AFM structure, in analogy to TbMnO$_3$. At T$_C$ = 30K the magnetic structure changes to weak ferromagnetism, attributed to a cone-like structure that breaks inversion symmetry and gives rise to ferroelectricity with the polarization along the a-axis.

We have investigated Eu$_{0.8}$Y$_{0.2}$MnO$_3$ using resonant x-ray diffraction as function of temperature, magnetic field and incident polarization at beamline P09 at PETRA III. The method of full polarization analysis has been used to investigate the different resonances showing up at the Mn K-edge. From the polarization scans, it is possible to draw conclusions on the complex magnetic order. Preliminary results suggest a helicoidal SDW structure of the Mn moments rather than a cone-like structure.

[1] J. Hemberger et al., Phys. Rev. B 75, 035118 (2007)

DS 3.4 Mon 10:15 H3

Electrostatic tuning of large-distance sputtered LSMO/PZT heterostructures — •Philipp Moritz Leufke, Ajay Kumar Mishra, Wang Di, Robert Kruk, and Horst Hahn — Institute of Nanotechnology (INT), Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany

In order to obtain a physical picture and quantitative characteristics of a magnetoelectric coupling at ferromagnetic/ferroelectric interfaces, epitaxial La$_{0.87}$Sr$_{0.13}$MnO$_3$/Pb(Zr,Ti)O$_3$ (LSMO/PZT) heterostructures were deposited by large-distance magnetron sputtering[1,2]. The remarkably high lateral uniformity achieved in such films allowed for a ferroelectric device area of more than 6 mm^2.

This has enabled for the first time *in-situ* SQUID measurements of the magnetic response to the systematically varied remanent ferroelectric polarization. Temperature dependence of the magnetic modulation upon charging and the magnetic response to the ferroelectric stimulation indicates a field-effect dominated coupling mechanism and generally confirms the concept of electrostatic hole (h^+) doping of LSMO.

For small charge modulations at low temperature, a linear tuning coefficient of $\approx 3.6\,\mu_\mathrm{B}/h^+$ has been determined. This suggests the activation of an antiferromagnetic coupling, even for very small surface charge densities. Simultaneously a shift in the magnetic transition temperature at higher surface charge concentration indicates the presence of a ferromagnetic phase at the LSMO/PZT interface.

[1] P. M. Leufke *et al.*, *Thin Solid Films* **520**, 5521 (2012).

[2] P. M. Leufke *et al.*, *AIP Advances* **2**, 032184 (2012).

DS 3.5 Mon 10:30 H3

Optimized magnetoelectric interface coupling — •Igor Maznichenko[1], Arthur Ernst[2], and Ingrid Mertig[1,2] — [1]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, D-06099 Halle (Saale), Germany — [2]Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle (Saale), Germany

It was shown that magnetoelectric coupling occurs at interfaces between a magnetic and a ferroelectric material. Our idea is to construct heterostructures with a particularly strong magnetoelectric coupling. We concentrate on the optimization of the magnetic layer. We demonstrate that a small magnetic moment at the interface can still transfer the magnetoelectric coupling to a strong ferromagnet and could cause significant response. The idea is supported by numerical simulations within density functional theory using the self-consistent KKR Green function method.

DS 3.6 Mon 10:45 H3

Role of electron correlation of FeO at Fe/ferroelectric oxide/Fe interface for magnetic transport properties — •Andrea Neroni, Daniel Wortmann, Ersoy Sasioglu, Stefan Blügel, and Marjana Ležaić — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

Fe/ferroelectric oxide/Fe is a nanoferronic tunnel junction with exciting electronic magneto-conductive transport properties. FeO layers at the interface of Fe/oxide/Fe barriers seems to significantly alter these properties as indicated by several experiments. In order to understand the role of electron correlations in FeO at the interface on the tunneling properties of a Fe/BaTiO$_3$/Fe barrier we use an embedded Green-function approach [1] implemented within the framework of the full-potential linearized augmented plane-wave (FLAPW) method `FLEUR` [2]. Conductances are obtained for different oxidation conditions and for different magnetic configurations of the contacts. Strong correlations are taken into account employing the LDA+U approach within the framework of the density functional theory (DFT) with a Hubbard U parameter determined by constrained random phase approximation (cRPA) [3]. Work is supported by Helmholtz Young Investigators Group Program VH-NG-409.

[1] www.flapw.de

[2] D. Wortmann, H. Ishida, and S. Blügel, PRB **65**, 165103 (2002)

[3] E. Şaşıoğlu, C. Friedrich, and S. Blügel, PRB **83**, 121101(R) (2011)

DS 3.7 Mon 11:00 H3

Multiferroic Aurivillius Phases: the Case of Bi$_5$FeTi$_3$O$_{15}$ by *ab initio* — •Yael Birenbaum, Nicola Spaldin, and Claude Ederer — Materials Theory, ETH Zürich, Switzerland

The Aurivillius phases form a family of naturally-layered perovskite-related materials with good ferroelectric properties. Bi$_5$FeTi$_3$O$_{15}$ (BFTO) is perhaps the simplest known member of this family that also incorporates magnetic degrees of freedom. Using *ab initio* electronic structure calculations, we establish the ferroelectric and magnetic properties of BFTO. We then discuss a possible site preference of the Fe^{3+} cation, which so far has not been found experimentally, and quantify the magnetic coupling between adjacent Fe cations. In addition, we analyse the different structural distortions, in order to relate BFTO to other members of the Aurivillius phases.

DS 3.8 Mon 11:15 H3

Strain effect on magnetic properties of La$_{0.7}$ Ca$_{0.3}$MnO$_3$/SrRuO$_3$ Superlattices — •Sujit Das[1,2], Andreas Herklotz[1,2], and Kathrin Doerr[1,2] — [1]IFW Dresden, Postfach 270116, 01171 Dresden, Germany — [2]Institute for Physics, MLU Halle-Wittenberg, 06099 Halle, Germany

Coherent interfaces between magnetic oxides such as La$_{0.7}$ Sr$_{0.3}$MnO$_3$ and SrRuO$_3$ may induce an intense magnetic coupling [1]. Recent work indicated an impact of elastic strain on the strength and even the sign of the coupling [2]. Superlattices (SL) of La$_{0.7}$ Ca$_{0.3}$MnO$_3$/SrRuO$_3$ with layer thicknesses below 10 unit cells were grown by pulse laser deposition simultaneously on SrTiO$_3$(001) (STO), LaAlO$_3$(001) (LAO) and piezoelectric 0.72Pb(Mg$_{1/3}$Nb$_{2/3}$)O$_3$-0.28PbTiO$_3$ (001) (PMN-PT) substrates and structurally characterized by X-ray diffraction (XRD). On LAO, the SL assumes a compressive strain state, i. e. the lattice parameter is larger out-of-plane than in-plane, whereas on PMN-PT it shows a tensile strain state and on STO an intermediate strain value. Magnetization measurements demonstrate a strong antiferromagnetic (AFM) coupling in SLs on STO and LAO substrates which is due to superexchange interaction between Ru and Mn ions. The AFM coupling seems to decrease under tensile strain. The coupling is much weaker on PMN-PT, probably because of higher interface roughness. In order to probe the effect of elastic strain directly, magnetization loops in reversibly controlled strain states have been recorded for SLs on PMN-PT. [1] M. Ziese et al., PRL 104, 167203 (2010), [2] J. W. Seo et al., PRL 105, 167206 (2010) .

DS 3.9 Mon 11:30 H3

Tuning the multiferroic phase of CuO with impurities — •Johan Hellsvik[1], Marcello Balestieri[1], Alessandro Stroppa[2], Anders Bergman[3], Lars Bergqvist[4], Olle Eriksson[3], Silvia Picozzi[2], and José Lorenzana[1] — [1]ISC-CNR, Rome, Italy — [2]CNR-SPIN, L'Aquila, Italy — [3]Uppsala University, Uppsala, Sweden — [4]KTH, Stockholm, Sweden

The discovery that CuO is a multiferroic with a high antiferromagnetic transition temperature of 230 K opened a possible route to room-temperature multiferroicity with a strong magnetoelectric coupling [1]. CuO belongs [2] to a new class of multiferroic materials where the so called 'order by disorder mechanism' [3] plays a crucial role. In this work we study the effect of different impurities on the phase diagram of CuO aiming at engineering the multiferroic properties. Extensive density functional theory (DFT) calculations were performed for a large number of fixed spin configurations in pure CuO and CuO doped with a small fraction of the Cu atoms substituted with the nonmagnetic elements Mg, Zn or Cd, or the magnetic elements Ni or Co. Our computations established that the energy difference between the low-temperature collinear AF1 phase and the intermediate temperature multiferroic AF2 phase decreased monotonously with increasing doping level confirming that impurities favour the multiferroic phase. The magnetic phase diagram has been mapped out in Monte Carlo simulations for classical Heisenberg spins. [1] T. Kimura et al., Nature Mat. 7, 291 (2008); [2] G. Giovannetti et al., Phys. Rev. Lett. 106, 026401 (2011); [3] C. L. Henley, Phys. Rev. Lett. 62, 2056 (1989)

DS 3.10 Mon 11:45 H3

Charge-mediated magnetoelectric coupling in patterned multiferroic heterostructures — •daniele preziosi[1], dietrich hesse[1], marin alexe[1], martin wahler[2], and georg schmidt[2] — [1]Max-Planck-Institut für Mikrostrukturphysik Weinberg 2, 06120 Halle(Saale) Germany — [2]Martin-Luther-Universität Halle-Wittenberg Von-Danckelman-Platz 3, 06120 Halle(Saale) Germany

Several studies on single phase multiferroics demonstrate that the coupling between the ferroelectric and the (ferro)magnetic order parameters tends to be small. Engineering of artificially structured systems could provide a reliable way to improve the MagnetoElectric (ME) coupling. Devices based on charge-mediated ME effect represent a viable alternative. The electric field produced by the polarization of the ferroelectric material can induce, at the interface with an ultrathin strongly correlated magnetic oxide, a change in the magnetization. The ME coupling would be in this case the consequence of the spin-dependent screening of the electric field. Patterned hetero-structures of La1-xSrxMnO3 (LSMO) and PbZr0.2Ti0.8O3 (PZT) have been fabricated. Transport and magnetic measurements show that the switching of the PZT polarization influences significantly the competing electronic ground states of the LSMO, modulating the resistivity as well as the magnetization value.

DS 4: Atomic Layer Deposition

Time: Monday 12:15–13:00 Location: H8

DS 4.1 Mon 12:15 H8

Realization of platinum 3D nanostructures using an improved atomic layer deposition process — •Yan Mi, Liaoyong Wen, ChengLiang Wang, Huaping Zhao, and Yong Lei — Fachgebiet 3D-Nanostrukturierung, Institut für Physik & IMN MacroNano (ZIK), Technische Universität Ilmenau, Prof. Schmidt Str. 26, 98693 Ilmenau, Germany.

Uniform deposition of metals onto high surface area of porous media is a key challenge for developing efficient catalysts and conducting layers. Self-limiting atomic layer deposition (ALD) provides excellent capabilities for depositing materials on large surface area. In this talk, we explored innovative three-dimensional (3D) surface nano-structuring technique to synthesize highly ordered functional nano-patterns with wide potential applications. The surfaces of as-prepared 3D nanostructures were further functionalized with platinum by ALD. Before the ALD process, the sample surface was modified by O2 plasma process. It is found that plasma-assisted ALD process intensively enhanced the quality of platinum, resulting in well-dispersed platinum nanoparticles and homogeneous continuous platinum nanotubes on highly ordered 3D nano-pattern surface. All these structural advantages make these 3D nanostructures highly desirable for catalysts and conducting layers.

DS 4.2 Mon 12:30 H8

Atomic layer deposition of Ga2O3 using Tri-methyl-Gallium and H2O — •Sakeb Hasan Choudhury, Massimo Tallarida, Chittaranjan Das, and Dieter Schmeisser — Brandenburg University of Technology, Applied Physics-Sensors technology, Konrad-Wacshmann-Allee, 17, 03046 Cottbus, Germany

Considering numerous applications such as transparent conducting oxides, gas sensors, photovoltaic applications, deep UV photo detectors, field effect transistors and spintronics gallium oxide (Ga2O3) has earned quite a lot of focus recently. Various techniques have already been demonstrated to produce Ga2O3 naming evaporation, sputtering, pulsed laser deposition, chemical vapor deposition and atomic layer deposition (ALD). Among them, ALD gives the possibility of controlling the thickness at the atomic level, good step coverage and delivers dense and homogeneous films. In this contribution, we report on the growth of ALD Ga2O3 using trimethylgallium (TMG) and H2O as metal and oxygen precursors, respectively. We deposited thin Ga2O3 films on Si, TiO2, Al2O3 and RuO2 over a temperature range of 150-300°C and characterized them by X-ray photo emission spectroscopy and atomic force microscopy. From this study, we are able to discuss the influence of the temperature on the growth dynamics of Ga2O3 and its chemical composition.

DS 4.3 Mon 12:45 H8

An efficient Si photo cathode for a wide range of electrolyte pH values — •Chittaranjan Das[1], Massimo Tallarida[1], Katarzyna Skorupska[2], Hans-Joachim Lewerenz[2,3], and Dieter Schmeisser[1] — [1]Applied physics and sensors,BTU Cottbus, Germany — [2]Institute for Solar Fuels and Energy Storage Materials,HZB, Berlin , Germany — [3]California Institute of Technology, 1200 East California, Pasadena , USA

Hydrogen fuel cells, being environmental friendly to produce energy, are a technology of future. One of the efficient ways to produce hydrogen is solar driven photocatalysis using semiconducting materials as photo electrodes. The choice of electrodes is a crucial factor and is done on the basis of photo corrosion stability, light absorption efficiency, and photocarrier lifetime. P-type Si can be used as photo cathode to produce H2 by direct photocatalysis. Si cathodes can be used in acidic electrolytes to have efficient photo catalytic activity but they are unstable in alkaline electrolytes. Therefore, to use both Si electrodes in the same electrolyte, their chemical stability should be extended over a wide range of pH. To this purpose we modified the surface of a p-type Si photocathode with very thin films of TiO2 grown by atomic layer deposition (ALD). We found that the modified Si cathode shows an increased photoresponse and a lower onset potential with respect to the pristine surface and an increased stability at various pH values.

DS 5: Charge Transfer Effects in Molecular Materials I (jointly with BP, CPP, HL)

Related to SYCT organized by Frank Schreiber (Tübingen) and Wolfgang Brütting (Augsburg).

Time: Monday 12:15–13:30 Location: H1

DS 5.1 Mon 12:15 H1

Thermally Activated Intermixing in Pentacene - Perfluoropentacene Heterostructures — •Tobias Breuer and Gregor Witte — Molekulare Festkörperphysik, Philipps-Universität Marburg, Renthof 7, 35032 Marburg

We report on the thermal stability of pentacene (PEN, $C_{22}H_{14}$) and perfluoropentacene (PFP, $C_{22}F_{14}$) heterostructures. We show that the thermal stability of the heterostructure compared to the single compounds is significantly enhanced by about 20 K. By varying preparation methods and stochiometric ratios of the heterostructures we show that the stabilization is restricted to heterostructures with stochiometric ratio of 1:1. Moreover, the thermal stabilization strongly depends on the preparation method, especially the deposition sequence of both materials in subsequent stacks. While PFP as bottom and PEN as top layer yield stabilized layers, no such effect is found for PEN as bottom layer and PFP on top. This asymmetry of intermixing and corresponding morphological information obtained by means of AFM measurements as well as optical absorption spectra as benchmark for hetero-interaction are discussed. The results are compared to additional preparation methods of heterostructures like co-evaporation and post-deposition-annealing.

DS 5.2 Mon 12:30 H1

Mixing-induced anisotropic correlations in molecular crystalline systems: Rationalizing the behavior of organic semiconductor blends — •Katharina Broch, Antje Aufderheide, Jiří Novák, Alexander Hinderhofer, Rupak Banerjee, Alexander Gerlach, and Frank Schreiber — Universität Tübingen, Institut für Angewandte Physik, Auf der Morgenstelle 10, 72076 Tübingen

Binary mixtures of organic semiconductors (OSCs) have recently become an important field of research, as they find applications in optoelectronic devices [1]. In these systems, the mixing (intermixing vs. phase separation) and ordering behavior is crucial, since it affects the optical and electronic properties including the degree of charge-transfer (CT). We present a comprehensive study of binary mixtures of the three prototypical OSCs pentacene (PEN), perfluoropentacene (PFP) and diindenoperlyene (DIP) in all possible combinations [1,2,3]. Using X-ray reflectivity and grazing incidence X-ray diffraction we investigate the structural properties of the mixed films as well as their impact on the optical spectra obtained by spectroscopic ellipsometry. For PEN:DIP we find an anisotropic ordering behavior, comparable to that observed in some liquid crystals, which is fundamentally new for OSCs [2]. The influence of sterical compatibility and the strength of the intermolecular interactions on the mixing and ordering behavior in the different blends will be discussed by extending a conventional mean-field model [1]. [1] A. Hinderhofer and F. Schreiber, Chem.Phys.Chem., **13**, 628 (2012); [2] A. Aufderheide et al., Phys.Rev.Lett., **109**, 156102 (2012); [3] J. Reinhardt et al., J.Phys.Chem. C, **116**, 10917 (2012)

DS 5.3 Mon 12:45 H1

Screening Effects on Excitation Energy Transfer in Supramolecular Complexes in a Mixed Quantum Classical Description — •Jörg Megow[1], Thomas Renger[2], and Volkhard May[1] — [1]Humboldt-Universität zu Berlin, Deutschland — [2]Johannes Kepler Universität Linz, Österreich

Excitation energy transfer (EET) within the supramolecular complex P16 (sixteen pheophorbide a molecules covalently linked to a DAB-dendrimer) is studied using a mixed quantum classical methodology [1,2] that takes the screening of excitonic coupling into acount. The excitonic coupling between two chromophores is calculated as Coulomb-coupling between transition partial charges. This treatment neglects the screening effects due to interaction with the solvent molecules. The Poisson-TrEsp (transition charges from electrostatic potentials) method [3], developed in the group of Renger, allows the calculation of screening factors that correct the excitonic coupling between two chromophores dependent on their distance, mutual orientation and conformation. A new method is proposed that allows to obtain the orientation and conformation dependence of the Poisson-TrEsp screening factors in a mixed quantum-classical description by introducing a novel fitting procedure. While all screening ansatzes result in a deceleration of the EET, the new approach results in a considerable acceleration of the EET compared to standard screening approaches.

[1] J. Megow et al., ChemPhysChem 12, 645 (2011) [2] J. Megow et al., Chem. Phys. 377, 10 (2010) [3] J. Adolphs et al., Photosynth. Res. 95 (2008)

DS 5.4 Mon 13:00 H1

In operando STXM investigations of charge carriers in SAMFET devices — •Andreas Späth[1], Thomas Schmaltz[2], Benjamin Watts[3], Marcus Halik[2], and Rainer H. Fink[1] — [1]FAU Erlangen-Nürnberg, Physical Chemistry II, Erlangen, Germany — [2]FAU Erlangen-Nürnberg, Polymer Sciences, Erlangen, Germany — [3]Swiss Light Source, Paul Scherrer Institut, Villigen, Switzerland

Based on previous work on pentacene based organic FETs [1], we present first results of zone plate scanning transmission soft x-ray microspectroscopy (STXM) on novel organic devices based on self assembled monolayers (SAMs). STXM combines high lateral resolution and spectroscopic sensitivity. Electron detection is used to achieve surface sensitivity, thus offering access to monolayer films. The SAMs implement all functionalities of the FET, i.e. gate dielectric and organic semiconductor [2]. STXM analysis within the active channel during operation of the SAMFET shows small variations in the electronic structure which are interpreted in terms of field induced shifts of the electronic levels and/or local charges. The unique combination of STXM and AFM provided by the NanoXAS beamline at the Swiss Light Source enables us to monitor both, the morphological homogeneity of the SAM film and modifications in the electronic structure. Thus, a more detailed insight into the correlation of morphological and electronic properties of these ultrathin devices can be achieved. The project is funded by the BMBF (contract 05K10WEA).

[1] C. Hub, et al., J. Mater. Chem. 20, 2010, 4884

[2] A. Rumpel, et al., Langmuir 27, 2011, 15016

DS 5.5 Mon 13:15 H1

Scanning Kelvin Probe Microscopy on FIB-milled Cross Sections of Organic Solar Cells — •Rebecca Saive[1,2,3], Christian Müller[1,2,3], Michael Scherer[1,2,3], Dominik Daume[1,2,3], Michael Kröger[1,3], and Wolfgang Kowalsky[1,2,3] — [1]InnovationLab GmbH, Heidelberg, Germany — [2]Kirchhoff-Institut für Physik, University Heidelberg, Germany — [3]Institut für Hochfrequenztechnik, Technische Universität Braunschweig, Germany

Scanning Kelvin probe microscopy (SKPM) is a promising tool to analyze charge carrier transport paths in electronic devices. Conventional SKPM is limited to analysis of charge transport parallel to the device surface, e.g. within planar field-effect transistors, whereas the transport in vertical devices e.g. bulk heterojunction solar cells is not accessible to further characterization. Therefore we introduce a method to directly measure at the cross sections of organic devices by milling with a focused ion beam (FIB) and adjacent SKPM characterization. By this method we can reveal a spatially resolved potential distribution and therefore indentify charge injection and charge transport barriers. In this work, we could correlate microscopic measurement results like the work function difference between the contact materials to macroscopic device characteristics received by J-V measurements and impedance spectroscopy.

DS 6: Focus Session: Ion Beam Induced Surface Patterns II

Time: Monday 14:45–16:00 Location: H8

DS 6.1 Mon 14:45 H8

Surface instability due to ion induced atomic mass transport - the CV model revisited — •Hans Hofsäss — II. Physikalisches Institut, Universität Göttingen

In this work the deterministic defining equations for the height evolution dh(x,y,t)/dt of a surface, originating from atomic mass redistribution parallel to the surface caused by ballistic displacements, are derived. The calculations follow the description of Carter and Vishnyakov [1] and Davidovitch et al. [2] but take into account important additional contributions to the height evolution not considered so far. Moreover, Monte Carlo simulations using SDTrimSP V5.05 [3] are used to derive ion incidence angle dependent quantities, like the recoil depth distribution and the lateral mean distance of atomic mass transport, from the calculated 3-dimensional recoil distributions. In this way simplified approximations of an angle dependence using a sine or cosine behaviour can be avoided. It will be shown that the transition from stability to instability in x-direction (parallel to the projected beam direction) is no longer fixed at 45°. Moreover, it will be shown, that in contrast to the conclusion in [2], ion-induced mass redistribution gives no contribution to stability or instability in y-direction.
[1] G. Carter, V. Vishnyakov, Phys. Rev. B 54, 17647 (1996).
[2] B. Davidovitch, MK. J. Aziz, M.P. Brenner, Phys. Rev. B 76, 205420 (2007).
[3] W. Eckstein, R. Dohmen, A. Mutzke, R. Schneider, MPI for Plasma Physics, IPP Report 12/3 (2007).

DS 6.2 Mon 15:00 H8

Ion beam induced surface patterns due to mass redistribution and curvature dependent sputtering — •Omar Bobes, Kun Zhang, and Hans Hofsäss — II. Physikalisches Institut, Universität Göttingen, Germany

We investigate the pattern formation on amorphous carbon films irradiated with 200 eV to 10 keV Xe ions. Sputter yield and number of displacements within the collision cascade vary strongly as function of ion energy and allow to investigate the contributions of curvature dependent erosion according to the Bradley-Harper model [1] and mass redistribution according to the Carter-Vishnyakov model [2]. We find parallel ripple orientations for 60° ion incidence angle and all energies. A transition to perpendicular patterns or a flat surface occurs around 80°. Our results are compared with calculations based on both models with parameters determined from simulations with program SDTrimSP [3]. The curvature coefficients S_x and S_y show that mass redistribution is dominant for parallel pattern formation. The angle where the parallel pattern orientation disappear is related to curvature dependent sputtering.
[1] R. M. Bradley and J. M. E. Harper, J. Vac. Sci. Technol. A6, 2390 (1988).
[2] G. Carter, V. Vishnyakov, Phys. Rev. B54, 17647 (1996).
[3] W. Eckstein, R. Dohmen, A. Mutzke, R. Schneider, MPI for Plasma Physics, IPP Report 12/3 (2007).

DS 6.3 Mon 15:15 H8

The role of phase separation for self-organized surface pattern formation by ion beam erosion and metal atom co-deposition — •Kun Zhang, André Pape, Omar Bobes, Marc Brötzmann, and Hans Hofsäss — II. Physikalisches Institut, Universität Göttingen, Germany

We investigate ripple pattern formation on Si during normal incidence ion beam erosion under simultaneous co-deposition of metallic surfactant atoms. In previous work on ion erosion of Si during co-deposition of Fe we proposed that chemical interactions between Fe and Si of the steady-state mixed Fe_xSi surface layer is a dominant contribution to self-organized pattern formation [1,2]. To generalize phase separation effects on the pattern formation we irradiated Si with normal incidence 5 keV Xe ions under simultaneous co-deposition of metal atoms. The metals in the two groups (Fe, Ni, Cu) and (W, Pt, Au) are similar regarding their collision cascade behaviour, but differ strongly regarding their tendency to silicide formation. We find pronounced pattern formation only for those metals which are prone to formation of mono- and disilicides. In contrast, for Cu and Au surfactants the surface remains very flat. Phase separation is seen as the relevant process for the pattern formation on Si during metal co-deposition.
[1] K. Zhang, M. Brötzmann, H. Hofsäss, New. J. Phys. 13, 013033 (2011).
[2] H. Hofsäss, M. Brötzmann, K. Zhang, AIP Advances 2, 032123 (2012).

DS 6.4 Mon 15:30 H8

Depth-resolved X-ray photoelectron and X-ray absorption spectroscopic study of Fe-implanted Si (100) — •behnam khanbabaee[1], stefan facsko[2], and ullrich pietsch[1] — [1]Universität Siegen, Festkörperphysik, 57072 Siegen, Germany — [2]Helholtz-zentrum Dresden-Rossendorf, 01314 Dresden, Germany

The bombardment of solid surfaces with energetic ions such as Ar+, Kr+ can be used for the fabrication of self-organized structures on surfaces. It was shown that different types of patterns on the nanoscale, i.e. dots, ripples and relief pattern can be generated by varying the experimental parameters. A number of experimental studies have shown that the simultaneously co-deposition of metal atoms like Fe during ion beam erosion has tremendous influence on pattern formation. Many aspects of the influence of co-deposited metal atoms are not fully understood. However, the formation of Fe-silicide is considered important for pattern formation on Si surfaces. In this work, we report on the formation of Fe-silicide in various phases after a direct, off-normal, ion implantation of 5 keV Fe+ ions on Si (100). A combination of X-ray photoelectron spectroscopy (XPS) and grazing incidence X-ray absorption spectroscopy (XAS) using synchrotron radiation were applied to clarify surface chemical states of Fe implanted Si. We found the formation of Fe-rich silicide (Fe3Si) in the near surface region, but the dominance of Si-rich silicide (FeSi2) in larger depth.

DS 6.5 Mon 15:45 H8

Tuning the uniaxial magnetic anisotropy of Fe thin films by using nano-rippled Si (100) substrates — •Sarathlal Koyiloth Vayalil[1], Ajay Gupta[2], and Stephan V. Roth[1] — [1]HASYLAB at DESY, Notkestr. 85, D-22603, Hamburg, Germany. — [2]UGC-DAE Consortium for Scientific Research, University Campus, Khandwa Road, Indore, India.

In this work, an alternative and effective way of tuning and tailoring the magnetic properties of Fe thin film by using nano-rippled Si(100) substrates prepared by low energy ion beam sputtering have been studied. The average wavelength and modulation depth of nano-rippled Si (100) substrate is in the order of 32 nm and 1.2 nm. Evolution of the magnetic properties of ultra thin Fe film on nano-rippled Si (100) substrate has been studied using in-situ MOKE measurements. Fe film on nanorippled Si surface exhibits a magnetic dead layer of 0.9 nm because of possible intermixing of Fe with Si to form non-magnetic silicide. It exhibits a strong uniaxial magnetic anisotropy with its easy axis along a direction normal to the ripple wave vector. The magnetic anisotropy is found to be decreasing with increasing film thickness. From the insitu resistivity measurements done simultaneously along and normal to the ripple wave vector shows, a clear anisotropy in the growth behavior along and normal to the ripple wave vector. Atomic force microscopy and GISAXS measurements on Fe thin films with different thicknesses shows that, initially the film conforms the morphology of the rippled substrate and later it vanishes.

DS 7: Multiferroics 2 (jointly with DF, KR, MA, TT)

Time: Monday 15:00–18:30 Location: H3

DS 7.1 Mon 15:00 H3

Magnetization control in thin two-phase multiferroic structures via external electric fields — •Alexander Sukhov[1], Paul P. Horley[2], Chenglong Jia[3], and Jamal Berakdar[1] — [1]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, D-06120 Halle/Saale, Germany — [2]Centro de Investigation en Materiales Avanzados, S.C. (CIMAV), 31109 Chihuahua, Mexico — [3]Key Laboratory for Magnetism and Magnetic Materials of the Ministry of Education, Lanzhou University, Lanzhou 730000, China

We present a theoretical study of the coupled magnetization and polarization dynamics in a thin multiferroic junction related to a $BaTiO_3$ (rhombohedral phase) layer in contact with Fe-layer. The dynamical properties are discussed in the context of different interfacial magnetoelectric coupling mechanisms. For the magnetoelectric coupling induced by the screening of the spin-polarized electrons in Fe we investigate the minimum strength of the coupling constant which is required for the full switching of the magnetization [1]. In the case of a strain-induced magnetoelectric interaction we show an electric field-induced magnetic switching in the plane perpendicular to the magneto-crystalline easy axis while the total magnetization remains stable [2]. In addition, the response of the multiferroic structure to magnetic radio-frequency fields by means of ferromagnetic resonance and dependent on the applied electric field is studied. [1] P.P. Horley, A. Sukhov, C.-L. Jia, E. Martinez, J. Berakdar, Phys. Rev. B **85**, 054401 (2012). [2] C.-L. Jia, A. Sukhov, P.P. Horley, J. Berakdar, Europhys. Lett. **99**, 17004 (2012).

DS 7.2 Mon 15:15 H3

Magnetic field induced charge anisotropy in $CoFe_2O_4$/$BaTiO_3$ nanocomposite — •Carolin Schmitz-Antoniak[1], Detlef Schmitz[2], Sven Stienen[1], Pavel Borisov[3], Anne Warland[1], Bernhard Krumme[1], Wolfgang Kleemann[1], and Heiko Wende[1] — [1]Fakultät für Physik, Universität Duisburg-Essen, D-47048 Duisburg — [2]Helmholtz-Zentrum Berlin für Materialien und Energie, D-12489 Berlin — [3]Department of Chemistry, University of Liverpool, Liverpool L69 7ZD

The system of $CoFe_2O_4$ nanopillars in a $BaTiO_3$ matrix represents a multiferroic nanocomposite in which strong ferrimagnetism and strong ferroelectricity coexist at room temperature [1]. The magnetostrictive CFO nanopillars and the piezoelectric BTO matrix are coupled by strain so that it is possible to change the electric properties by a magnetic field and the magnetic properties by an electric field. The charge anisotropy of Ti ions is probed by x-ray linear dichroism (XLD) and the magnetisation of Co ions by x-ray magnetic circular dichroism (XMCD) giving the unique possibility to study the effect of the coupling on a microscopic level as a function of magnetic field strength and direction. The occurrence of significant in-plane components of the electric polarisation is discussed. They are due to shear forces acting on the $BaTiO_3$ matrix while taking into account non-diagonal piezoelectricity components.

Funded by DFG (SFB491) and BMBF (05 ES3XBA/5).

[1] H. Zheng et al., Science 303, 661 (2004)

DS 7.3 Mon 15:30 H3

Multiferroic CoFe2O4/ BaTiO3 with core shell structure nanoparticles — •Morad Etier[1], Vladimir V.Shvartsman[1], Yanling Gao[1], Joachim Landers[2], Heiko Wende[2], and Doru C.Lupascu[1] — [1]University of Duisburg-Essen, Institute for Materials Science, Essen, Germany — [2]University of Duisburg-Essen, Faculty of Physics, Duisburg, Germany

Multiferroic materials exhibit ferroelectricity and ferromagnetism simultaneously. Combining piezoelectricity and magnetostriction components in the same composite received more interests in the modern researches. In this work we report synthesis and properties of cobalt iron oxide barium titanate composite with a core shell structure. To synthesize the samples we combine co-precipitation and organosol method. Phases content, microstructure and morphology were studied by x-ray diffraction, SEM and TEM. Multiferroic properties were proved by home-built Sawyer-Tower circuit and SQUID magnetometry. Temperature dependence of magnetic moment was measured in zero field cooling (ZFC) and field cooling (FC) and compared with those cobalt iron oxide nanopowder. The dielectric properties were studied using impedance spectroscopy.

DS 7.4 Mon 15:45 H3

Strain-induced changes of magnetic anisotropy in epitaxial spinel-type cobalt ferrite films — •Stefania Florina Rus[1,2], Andreas Herklotz[2,4], Iuliu Grozescu[3], and Kathrin Dörr[4] — [1]Politehnica University of Timişoara, 300006 Timişoara, Romania — [2]IFW Dresden, 01171 Dresden, Germany — [3]Institute for Research and Development in Electrochemistry and Condensed Matter, 300224 Timisoara, Romania — [4]Martin-Luther-Universität Halle-Wittenberg, Institute for Physics, 06099 Halle, Germany

We present results on the effect of biaxial strain on the magnetic anisotropy of thin films of the parent compound CoFe2O4 and films with a partial substitution of Co and Fe by Zr and Pt, respectively. The strain states of the epitaxially grown films are controlled twofold: (i) statically by epitaxial misfit strain via an appropriate choice of substrates and buffer layers and (ii) reversibly by strain transfer from piezoelectric $Pb(Mg_{1/3}Nb_{2/3})_{0.72}Ti_{0.28}O_3$ (001) (PMN-PT) substrates. Due to large negative magnetostriction all films show an out-of-plane magnetic easy axis under tensile strain and an in-plane easy axis under compressive strain. Our reversible strain measurements show that the magnetic anisotropy can be efficiently altered by the application of an electric field to the ferroelectric PMN-PT substrates. The effect of substitution with Zr and Pt on the magnetoelectric effect will be discussed. This work is supported by the strategic grant POSDRU ID77265 (2010), co-financed by the European Social Fund, within the Sectoral Operational Programme Human Resources Development 2007-2013. Advising by P. Vlazan is greatly acknowledged.

DS 7.5 Mon 16:00 H3

***Ab initio* study of magneto-phonon interaction in $GaFeO_3$** — •Konstantin Z. Rushchanskii, Stefan Blügel, and Marjana Ležaić — Peter Grünberg Institut, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

Magnetoelectric (ME) coupling provides a handle for manipulating the magnetization of a material with an electric field, giving a perspective for a new type of non-volatile memory. Unfortunately, materials with ME coupling that is large enough for industrial applications are scarce. Moreover, among the materials which are both ferroelectric and magnetic at room temperature, only $BiFeO_3$ is known. Unfortunately, the ordering of spins in this material is antiferromagnetic (whereas ferro/ferrimagnetic coupling is desired) and the ME coupling is small.

$GaFeO_3$ (GFO) is the first material observed to simultaneously present a strong ME coupling and a resulting magnetization in a single phase. It has the polar structure $Pc2_1n$, which allows disorder in A and B cation sites. By increasing the iron content its Curie temperature can be increased above room temperature [1].

To understand the mechanism of the strong ME coupling in $GaFeO_3$ at the microscopic level, we performed *ab initio* calculations based on density functional theory of the structural properties and magneto-phonon interaction in stoichiometric $GaFeO_3$ compounds in different structures, as well as with different occupancies of the A and B sites.

We acknowledge the support by Helmholtz Young Investigators Group Programme VH-NG-409 and GALIMEO Consortium.

[1] T. Arima *et al.*, Phys. Rev. B **70**, 064426 (2006)

DS 7.6 Mon 16:15 H3

The effect of ion doping on multiferroic $MnWO_4$ — •safa golrokh bahoosh[1,3], julia m. wesselinowa[2], and steffen trimper[3] — [1]Max Planck Institute of Microstructure Physics,Weinberg 2, 06120 Halle, Germany — [2]University of Sofia, Department of Physics,Blvd. J. Bouchier 5, 1164 Sofia, Bulgaria — [3]Institute of Physics, Martin-Luther-University, 06120 Halle, Germany

We have studied the ion doping effects on different transition temperatures in the multiferroic compound $MnWO_4$ based on a microscopic model and within the framework of Green functions technique. It is shown that the exchange interaction constants can be changed due to the different ion doping radii. This leads to reduction of the magnetic phase transition temperature T_N by doping with non-magnetic ions,such as Zn, Mg, whereas T_N is enhanced by doping withtransition metal ions, such as Fe, Co. The different behavior of the temperature T_1 (where up-up-down-down collinear spin structure appears) by Fe and Co doping could be explained taking into account the single-ion anisotropy.

15 min. break

DS 7.7 Mon 16:45 H3

Hybrid improper ferroelectricity in a Multiferroic and Magnetoelectric Metal- Organic Framework — •Alessandro Stroppa[1], Paolo Barone[1], Prashant Jain[2], Manuel Perez-Mato[3], and Silvia Picozzi[1] — [1]CNR-SPIN Via Vetoio, 67100, L'Aquila (Italy) — [2]Los Alamos National Lab, 30 Bikini Atoll Rd Los Alamos, NM 87545-0001 (505) 664-5265 — [3]Departamento de Fisica de la Materia Condensada, Facultad de Ciencia y Tecnologia, UPV/EHU, Bilbao (Spain)

Metal-organic frameworks (MOFs) show increasing promise as candidates for various applications. Of particular interest are MOFs with the perovskite topology showing hydrogen bonding-related multiferroic phenomena. By using state-of-the-art-ab-initio calculations, we show that in [C(NH2)3]Cr(HCOO)3 MOF, interaction between the cooperative antiferro-distortive Jahn-Teller distortions and the C(NH2)3 cations breaks the inversion symmetry through hydrogen-bonding and induces a ferroelectric polarization. Interestingly, the polar behavior arises due to a trilinear coupling between two unstable modes, namely a Jahn-Teller and a tilting mode, and one stable polar mode. Therefore, this compound represents the first example of hybrid improper ferroelectric in the family of metal-organic compounds. Since rotational modes in perovskite-inorganic compounds usually freeze-in at elevated temperatures (300 K), the trilinear coupling in MOF compounds may provide an interesting route to realize room temperature multiferroic. Last but not least, we show that switching of polarization direction implies the reversal of a large weak ferromagnetic component.

DS 7.8 Mon 17:00 H3

Ferroelectric properties of (Ba,Sr)TiO$_3$/La$_{0.7}$Sr$_{0.3}$MnO$_3$ multilayered thin films — •Markus Michelmann[1], Johannes Aprojanz[1,2], Arseni Buryakov[2], Elena Mishina[2], Markus Jungbauer[1], Sebastian Hühn[1], and Vasily Moshnyaga[1] — [1]I. Physikalisches Institut, Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen — [2]Moscow State Institute of Radioengineering, Electronics and Automation, Prosp. Vernadskogo 78, 119454 Moscow, Russia

Ba$_x$Sr$_{1-x}$TiO$_3$ (BSTO) epitaxial thin films became feasible for room temperature applications in contrast to the bulk material due to a possibility to enhance the ferroelectric Curie temperature under biaxial compressive strain. Using La$_{0.7}$Sr$_{0.3}$MnO$_3$ (LSMO) thin films as metallic electrodes, we have grown highly strained BSTO/LSMO bilayers and LSMO/BSTO/LSMO trilayers on SrTiO$_3$ (100) substrates with BSTO layer thicknesses of 10 - 200 nm by means of metalorganic aerosol deposition. Ferroelectric switching was studied both electrically and by nonlinear optics (second harmonic generation (SHG)). Capacitance-voltage characteristics in a frequency range of $f = 1-10^6$ Hz and PUND measurements prove a ferroelectric hysteretic behavior up to room temperature with a remanent polarization of several $\mu C/cm^2$ and a switching fields in the range of $10-100$ kV/cm. This was also supported by the SHG measurements. A detailed study of multiferroic properties will be performed for temperatures, $T = 10-400$ K, and applied magnetic field, $B = 0-9$ T. This work was supported by IFOX of the European Community's 7th Framework Programme.

DS 7.9 Mon 17:15 H3

Epitaxial thin films of the multiferroic double perovskite Bi$_2$FeCrO$_6$ — •Vikas Shabadi, Mehran Vafaee, Mehrdad BaghaieYazdi, Aldin Radetinac, Philipp Komissinskiy, and Lambert Alff — Institute of Materials Science, Technische Universität Darmstadt, Germany

Co-existence of magnetism and ferroelectricity was theoretically predicted in the ordered double perovskite Bi$_2$FeCrO$_6$ (BFCO) [1]. We report epitaxial BFCO thin films grown by pulsed laser deposition from a 20% Bi-rich ceramic target on single crystal SrTiO$_3$(100) substrates. The degree of the Fe-Cr cation ordering in the BFCO films was calculated based on the X-ray diffraction patterns. The magnetic moments of the BFCO films were measured with a SQUID magnetometer and analyzed as a function of the Fe-Cr ordering. The discrepancies in the previously reported values of the magnetic moment of BFCO [2,3] are most likely connected to the varying degree of the Fe-Cr cation ordering in the samples. In a recent experiment more than 90% spontaneous B-site ordering in a similar Fe-Cr based double perovskite system has been achieved [4]. Anti-site disorder control is a key challenge to design double perovskite multiferroics.

[1]P. Baettig and N. A. Spaldin, Appl. Phys. Lett. **86**, 012505 (2005)

[2]Kim *et al.*, Appl. Phys. Lett. 89, 102902 (2006)

[3]R. Nechache *et al.*, J. Appl. Phys. **105**, 061621 (2009)

[4]S. Chakraverty *et al.*, Phys. Rev. B **84**, 064436 (2011)

The authors acknowledge support from DAAD.

DS 7.10 Mon 17:30 H3

Growth of multiferroic heterostructures — •Sergiu Stratulat, Dietrich Hesse, and Marin Alexe — Max-Planck-Institut für Mikrostrukturphysik, Halle, Germany

Coupling two materials with different order parameters gives great flexibility in engineering multifunctional devices. In achieving the maximum interfacial effects, vertical heterostructures present the maximum potential. Creating well-ordered vertical multiferroic heterostructures is not a trivial task, especially on large areas. We are focusing our attention on the system comprising ferrimagnetic CoFe2O4 and ferroelectric/antiferromagnetic BiFeO3, using pulsed laser deposition as a synthesizing technique. Considering a time-viable process to create the pillar-matrix configuration, we used anodic aluminum oxide masks to pattern the nucleation sites for the cobalt ferrite on previously deposited SrRuO3 bottom electrode on SrTiO3. After removal of the mask, deposition by means of a mixed target leads to ordered arrays of CFO pillars embedded in a BFO matrix. Scanning electron microscopy was employed at every step of the experiments to show the development of the samples, and X-ray diffraction probed the structural parameters. Testing the ferroelectric and magnetic properties locally gives an indication on the coupling influences present in the thin films.

DS 7.11 Mon 17:45 H3

Self-assembled composite multiferroic films in controlled strain states — •Mohsin Rafique[1,2,3,4], Andreas Herklotz[3,4], Er-Jia Guo[3,4], Kathrin Doerr[3,4], and Sadia Manzoor[1,2] — [1]Magnetism Laboratory, COMSATS Institute of Information Technology, Park Road 44000, Islamabad, Pakistan — [2]Center for Micro and Nano Devices (CMND), COMSATS Institute of Information Technology, Park Road 44000, Islamabad, Pakistan — [3]IFW Dresden, Postfach 270116, 01171 Dresden, Germany — [4]Institute for Physics, Martin-Luther-University Halle-Wittenberg, 06099 Halle, Germany

Self-assembled thin-film nanocomposites of piezoelectric and magnetostrictive materials have stimulated increasing research activities because of their potential to exhibit a large magnetoelectric response exploitable in multifunctional devices. Epitaxial thin films of CoFe$_2$O$_4$ and BaTiO$_3$ (CFO-BTO) composites were grown on SrTiO$_3$ (001) and piezoelectric Pb(Mg$_{1/3}$Nb$_{2/3}$)$_{0.72}$Ti$_{0.28}$O$_3$(001) (PMN-PT) substrates by pulsed laser deposition. Self-assembled nanostructures consisting of spinel nanopillars heteroepitaxially embedded in the ferroelectric perovskite matrix form. X-ray diffraction is utilized to estimate the lattice parameters. The magnetic properties studied by SQUID magnetometry show an out-of-plane easy axis of the CFO nanopillars and a strengthening of the out-of-plane anisotropy with increasing compression along the nanopillar axis. The magnetoelectric coupling in the composite film is revealed at a structural transition of the BTO matrix. Electrically controlled substrate strain of PMN-PT is applied to modify the magnetic anisotropy of the nanopillars.

DS 7.12 Mon 18:00 H3

Low-lying magnetic excitations in the distorted triangular lattice antiferromagnet α-CaCr$_2$O$_4$ — •Michael Schmidt[1], Zhe Wang[1], Sandor Toth[2], Bella Lake[2], A.T.M.Nazmul Islam[2], Alois Loidl[1], and Joachim Deisenhofer[1] — [1]Experimental Physics V, Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, D-86135 Augsburg, Germany — [2]Helmholtz-Zentrum Berlin für Materialien und Energie, D-14109 Berlin, Germany

We will discuss our results on α-CaCr$_2$O$_4$ obtained by FIR and Terahertz spectroscopy. This compound orders below $T_{\mathrm{N}} = 42.6$ K in a proper screw 120° magnetic order, but shows additional low-lying magnetic modes indicative for the vicinity of a more complex magnetic order [1], [2]. Our spectra obtained by FTIR and THz-TD spectroscopy show several optical magnons appearing below the magnetic ordering with anomalous temperature dependence. We will discuss their polarization dependence and a possible magnetoelastic coupling of these modes.

[1] S. Toth *et al.*, Phys. Rev. B 84, 054452 (2011)
[2] S. Toth *et al.*, PRL 109, 127203 (2012)

DS 7.13 Mon 18:15 H3

Multiferroic $Ni_3V_2O_8$ measured in THz range at low temperatures and in high magnetic fields — •Malte Langenbach[1], Tobias Hissen[1], Komalavalli Thirunavukkuarasu[1], Holger Schmitz[1], Iván Cámara Mayorga[2], Rolf Güsten[2], Joachim Hemberger[1], and Markus Grüninger[1] — [1]II. Physikalisches Institut, Universität zu Köln, Köln, Germany; — [2]Max-Planck-Institut für Radioastronomie, Bonn, Germany;

THz spectroscopy in high magnetic fields is an important technique to probe materials with strong magneto-electric coupling. Here, we discuss the Kagomé-staircase compound $Ni_3V_2O_8$. The triangle-based lattice gives rise to a frustration of the short-range antiferromagnetic couplings. This causes a rich variety of magnetic and structural phases at low temperatures.
Below $T_N = 9.8$ K, a incommensurate phase with collinear sinusoidal spin structure is established. This phase is followed by a cycloidal spin structure which is accompanied by the onset of ferroelectricity. Finally, below 3.9 K, the structure changes to a commensurate canted antiferromagnetic phase [1].
We report on elementary excitations in the THz range observed between 2 K and 50 K in fields up to 8 T.

Work supported by the DFG through SFB 608.

[1] G. Lawes et al., Phys. Rev. Lett. **95**, 087205 (2005)

DS 8: Charge Transfer Effects in Molecular Materials II (jointly with BP, CPP, HL)

Related to SYCT organized by Frank Schreiber (Tübingen) and Wolfgang Brütting (Augsburg).

Time: Monday 15:00–17:30 Location: H40

Invited Talk DS 8.1 Mon 15:00 H40

a molecular picture of charge-transfer processes at donor-acceptor interfaces in organic solar cells — •Jean-Luc Bredas — School of Chemistry and Biochemistry/Center for Organic Photonics and Electronics, Georgia Institute of Technology, Atlanta, Georgia 30332-0400

Our objective in this presentation is two-fold. First, after a general introduction to organic solar cells, we use a molecular mechanics / molecular dynamics simulations approach to try and provide a molecular picture of the packing configurations (local morphology) at the interface between the donor and acceptor components in organic solar cells [1-3]. Then, we discuss in detail the impact that these local packing configurations at the interfaces have on the exciton-dissociation and charge-separation processes [4]. Systems under consideration include fullerene derivatives or n-type oligoacene derivatives as acceptors and low optical-gap polymers or small molecules (pentacene or squaraine derivatives) as donors.

References (1) N. Cates Miller, E. Cho, et al., Advanced Materials, in press (DOI: 10.1002/adma.201202293). (2) N. Cates Miller, E. Cho, et al., Advanced Energy Materials, in press (DOI: 10.1002/aenm.201200392). (3) Y.T. Fu, C. Risko, and J.L. Bredas, Advanced Materials, in press (DOI: 10.1002/adma.201203412). (4) J.L. Bredas, J. Norton, J. Cornil, and V. Coropceanu, Accounts of Chemical Research 42, 1691 (2009).

DS 8.2 Mon 15:30 H40

Microscopic simulations of charge transport in disordered organic semiconductors — •Denis Andrienko, Bjoern Baumeier, Pascal Kordt, Anton Melnyk, and Carl Poelking — Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany

Charge carrier dynamics in an organic semiconductor can often be described in terms of charge hopping between localized states. The hopping rates depend on electronic coupling elements, reorganization energies, and driving forces, which vary as a function of position and orientation of the molecules. The exact evaluation of these contributions in a molecular assembly is computationally prohibitive. Various, often semi-empirical, approximations are employed instead. Here, we review the current status of methods used to evaluate energetic disorder in organic semiconductors, such as polarizable force-fields and QM/MM approaches, focusing on their predictive power and accuracy. All methods are illustrated on donor-acceptor small-molecule interfaces as well as crystalline mesophases of conjugated polymers.

DS 8.3 Mon 15:45 H40

Metal-Molecule Charge Transfer through Surface-Induced Conjugation — •Georg Heimel[1], Steffen Duhm[2], Ingo Salzmann[1], Alexander Gerlach[3], Antje Vollmer[4], Frank Schreiber[3], and Norbert Koch[1] — [1]Institut für Physik, Humboldt-Universität zu Berlin, 12489 Berlin, Germany — [2]Institute of Functional Nano & Soft Materials, Soochow University, Suzhou 215123, P. R. China — [3]Institut für Angewandte Physik, Universität Tübingen, 72076 Tübingen, Germany — [4]Helmholtz Zentrum Berlin für Materialien und Energie GmbH, 12489 Berlin, Germany

For the majority of large π-conjugated molecules, the Fermi level of supporting coinage-metal substrates is *pinned* to stay well within their electronic energy gap. In some cases, however, the Fermi level *does* cross into either of the frontier molecular orbitals. On the basis of a combined multi-technique experimental and theoretical study on a particularly clear-cut case – pentacenequinone and pentacenetetrone on the (111) surfaces of Au, Ag, and Cu – we present an attempt for a unifying explanation of such intriguing cases: The conjugation length of the organic semiconductor increases through interaction of specific chemical substituents with the metal surfaces. The ensuing reduction of the energy gap is found to be *the* crucial ingredient needed to overcome Fermi-level pinning. Our findings aid in the design of charged molecular monolayers, which are of interest both from the fundamental- and the applied-physics point of view.

Invited Talk DS 8.4 Mon 16:00 H40

High efficiency OLEDs based on delayed fluorescence — •Chihaya Adachi — OPERA, Kyushu University, Fukuoka, Japan

We achieved a novel pathway to reach the ultimate EL efficiency by inventing simple aromatic compounds displaying efficient thermally-activated delayed fluorescence (TADF) with high photoluminescence efficiency, namely *hyperfluorescence*. While we had previously assumed that the S1 level should be significantly higher than the T1 level, i.e., 0.5˜1.0 eV higher, due to the presence of electron exchange energy, we found that the proper design of organic molecules can lead to a small energy gap (ΔEST) between them. Relatedly, a molecule displaying efficient TADF requires a very small ΔEST between its S1 and T1 excited states, resulting in enhanced T1 * S1 reverse intersystem crossing (ISC). Such excited states are attainable by the intramolecular charge transfer (CT) of a spatially separated donor and acceptor system. The critical point of the molecular design is the compatibility of a small ΔEST ˜ 0 eV and a reasonable radiative decay rate of over 106/s that overcomes competitive non-radiative decay paths, leading to highly luminescent TADF materials. Since the two properties conflict with each other, a delicate balance of the overlap of the highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) is required. Furthermore, to enhance the PL efficiency of a TADF material, geometrical change between its S0 and S1 states should be restrained to suppress non-radiative decay processes. In this work, we designed a novel series of highly efficient TADF emitters that resulted in very high electroluminescence efficiency.

DS 8.5 Mon 16:30 H40

Triplet Exciton Generation and Electron Back Transfer in Organic Solar Cells — •Andreas Sperlich[1], Hannes Kraus[1], Stefan Väth[1], Alexander Förtig[1], Carsten Deibel[1], and Vladimir Dyakonov[1,2] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — [2]ZAE Bayern, 97074 Würzburg

To increase the power conversion efficiency of organic solar cells it would be extremely advantageous to improve the harvesting of singlet and charge transfer (CT) excitons. Dissociation of CT complexes into free charge carriers or, alternatively, their decay by electron back transfer (EBT) reactions depend on the energy levels of constituting donor and acceptor molecules, on microscopic structure of blends but also on the relative spin orientation of charges carriers within the e-h pair. We report on state-of-the-art organic semiconductors for polymer-fullerene bulk hetero-junction solar cells, such as blends based on the benzodithiophene donor PTB7 or the endohedral fullerene-derivative $Lu_3N@C_{80}$-PCBEH. We applied optical, current-voltage, morphology, and spin-sensitive techniques and found correlations between electrical performance of solar cells and formation of CT and triplet states. Combining results of these complementary experiments, we offer a physical picture on how pushing up the LUMO level of acceptors or tailoring the blends' morphology may end up in unwanted loss mechanisms in bulk-heterojunction solar cells.

DS 8.6 Mon 16:45 H40

Reduced recombination and field independent charge carrier generation in polymer-polymer solar cells — •Steffen Roland[1], Marcel Schubert[1], Zhihua Chen[2], Antonio Facchetti[2], and Dieter Neher[1] — [1]University of Potsdam, Institute of Physics and Astronomy — [2]Polyera Corporation

Charge transport and recombination are investigated for solar cells made of poly(3-hexylthiphene) (P3HT) and the non-fullerene, high mobility acceptor copolymer P(NDI2OD-T2). Optimized devices show high fill factors of up to 70%, indicating that the excellent electron transport properties of pure P(NDI2OD-T2) is prevailed in the blend. By applying of the time delayed collection field technique (TDCF) we measured the field dependence of the charge carrier generation, and of the non geminate recombination as well as the electron and hole mobilities. The results reveal a field-independent photocurrent generation and a strongly reduced recombination coefficient for free charge carriers. The results imply that major charge carrier losses originate from an ultrafast (geminate) recombination on time scales below 10 ns.

Invited Talk DS 8.7 Mon 17:00 H40

The role of intermolecular hybridization in molecular electrical doping — •Ingo Salzmann[1], Georg Heimel[1], Henry Méndez[1], Andreas Opitz[1], Patrick Barkowski[1], Martin Oehzelt[2,1], Katrein Sauer[1], and Norbert Koch[1,2] — [1]Humboldt Universität zu Berlin — [2]Helmholtz Zentrum Berlin, Germany

Molecular electrical doping of functional organic semiconductor (OSC) films is typically done by the admixture of strong molecular donors/acceptors as dopants. In a recent combined experimental and theoretical study on prototypical OSC/dopant pairs we showed that positive polarons, evidencing the common perception of direct electron transfer between the highest occupied molecular orbital (HOMO) of the OSC and the lowest unoccupied molecular orbital (LUMO) of the p-dopant, are not observed in ultraviolet photoelectron spectroscopy even at considerable dopant ratios [1]. Instead of mutual ionization leading to singly occupied states, frontier molecular orbital hybridization between the OSC-HOMO and the dopant-LUMO occurs forming a *doubly occupied* bonding and an *empty* anti-bonding supramolecular hybrid orbital with a reduced fundamental gap, which is tunable by the acceptor strength. As all available states are occupied following Fermi-Dirac statistics, only a fraction of the hybrids is ionized at room temperature rationalizing the high dopant concentrations in practical applications. From this model, controlling the degree of hybridization emerges as strategy for the design of future improved molecular dopants in organic electronic devices.

[1] I. Salzmann, G. Heimel et al., *Phys. Rev. Lett.* 108, 035502, 2012.

DS 9: Ion and Electron Beam Induced Processes

Time: Monday 16:15–17:15 Location: H8

DS 9.1 Mon 16:15 H8

Sputtering effects on ion irradiated Au nanoparticles — •Henry Holland-Moritz[1], Christian Borschel[1], Sebastian Scheeler[2], Claudia Pacholski[2], and Carsten Ronning[1] — [1]Institut für Festkörperphysik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena — [2]Max-Planck-Institut für Intelligente Systeme, Heisenbergstrasse 3, 70569 Stuttgart

Today, nanoparticles can easily be fabricated by different physical and chemical processes and can also be arranged in many different patterns and shapes. However, the synthesis is usually restricted to thermally equilibrium conditions. Ion beam irradiation, a non-equilibrium method, is one possible subsequent approach to tune the properties of nanoparticles. An important effect in this case is sputtering, especially when the ion range in the nanoparticles material is in the range of its size. For different purposes, it is important to understand the quantity of the sputtering effects on nanoparticles and how sputtering works on nanoparticles on top of substrates due to enhanced sputtering in nanostructures compared to bulk-like structures or films. Simulations were done by the Monte-Carlo-code iradina and hexagonal arranged gold nanoparticles with diameters of 50 nm on top of silicon substrates with native oxide layer were irradiated by argon ions using energies from 20 keV up to 350 keV and different ion fluencies. The sputtering effects were investigated with SEM and AFM measurements to get information about the energy dependence of the sputteryield and the fluence dependence of the volume decrease of the nanoparticles and the results were compared with the simulation results by iradina.

DS 9.2 Mon 16:30 H8

Bombardment induced ion transport (BIIT) through thin polymer films — •Susanne Schulze, Julia Zakel, Martin Schäfer, Andreas Greiner, and Karl-Michael Weitzel — Philipps-Universität Marburg, FB Chemie, 35032 Marburg

We report on the transport of potassium ions (K^+) through Poly(*para*-xylylene) (PPX) films (thickness 100 nm to 2720 nm) induced by ion bombardment. The films were formed by plasma chemical vapor deposition onto a metal electrode. The experiments were performed in an UHV apparatus where an ion beam is generated by thermionic emission of potassium ions from aluminosilicates. By bombarding the PPX films with an ion beam of low kinetic energy (10 eV to 500 eV) we generate a potential gradient and a concentration gradient inducing transport of the ions through the material. The ion transport is detected as a current on the backside electrode of the film. By measuring this current as a function of the kinetic energy of the impinging ions, we are able to determine the ionic conductivity of the material. In a second experiment PPX is bombarded with an ion beam of constant kinetic energy for several days. This experiment leads to the formation of an electro-diffusion profile of potassium in the film as shown by time-of-flight secondary ion mass spectrometry. The potassium diffusion profiles, which reach through the entire film, can be quantitatively described by theoretical calculations based on the numerical solution of the Nernst-Planck-Poisson equations. From this analysis we conclude that the effective diffusion coefficient of K^+ in PPX decreases with increasing incorporation of the K^+ ions into the film.

DS 9.3 Mon 16:45 H8

The role of defect-types in ion beam induced stress in $LiNbO_3$ — •Emanuel Schmidt, Tobias Steinbach, and Werner Wesch — Institute of Solid State Physics, Friedrich Schiller University Jena

Ion-irradiation of complex crystalline materials, such as Lithium niobate ($LiNbO_3$), can result in the formation of different types of defects. With increasing ion-irradiation these defects accumulate or convert into more extensive defects, until in many materials a continuous amorphous surface layer is formed. This phase-transformation in general involves a density-change, which leads to the formation of mechanical forces. However, only a few quantitative studies on ion beam induced stress phenomena have been made, even though stresses in microstructures cause substrate bending, delamination and cracking as well as anomalous diffusion of dopands. To investigate the ion beam induced formation and relaxation of stress due to the formation and accumulation of defects and amorphous regions a scanning laser reflection technique was established at the FSU Jena. By means of this technique the bending of a freestanding sample away from the irradiated surface is defined by the compensation of forces and moments between the underlying substrate and the irradiated regions. In the case of $LiNbO_3$ these forces are highly anisotropic due to the crystal-structure of the material. The fluence dependent stress-evolution in $LiNbO_3$ shows a different behaviour compared to classical semiconductors, such as Ge and Si. The results are discussed in the framework of a defect-related model. Additional Rutherford-backscattering-measurements support the applied defect-relations in this approach.

DS 9.4 Mon 17:00 H8

Temperature- and orientation-dependent damage-formation due to electronic energy deposition in $LiNbO_3$ — •Matthias Schmidt[1], Jura Rensberg[1], Frank Schrempel[2], and Werner Wesch[1] — [1]Institute of Solid State Physics, Friedrich Schiller University Jena — [2]Institute of Applied Physics, Friedrich Schiller University Jena

Among the methods to realize micro- and nanostructures with high aspect ratio in order to fabricate novel photonic devices in $LiNbO_3$ crystals, ion beam enhanced etching (IBEE) was found one of the most promising techniques. The high ion energies (several MeV) necessary to achieve sufficiently deep structures (several μm) are accompanied by high electronic energy deposition dominating especially close to the sample surface.
It is well known that the ion fluences to produce damage and to amorphize the material in the electronic energy loss regime are at least an order of magnitude lower compared to the fluences necessary to produce the same damage concentration by means of nuclear energy deposition. In this contribution the damage evolution up to complete amorphization in $LiNbO_3$ was investigated using MeV oxygen and silicon ions. The transition to the amorphous phase was studied as a function of irradiation temperature and crystal orientation. The differences in damage formation due to nuclear and electronic processes are discussed.

DS 10: Organic Electronics and Photovoltaics I (jointly with CPP, HL, O)

Time: Monday 17:15–18:45 Location: H32

DS 10.1 Mon 17:15 H32

Correlation between interface energetics and open circuit voltage in organic photovoltaic cells — •Andreas Wilke[1], James Endres[2], Ulrich Hörmann[3], Jens Niederhausen[1], Raphael Schlesinger[1], Johannes Frisch[1], Patrick Amsalem[1], Julia Wagner[3], Mark Gruber[3], Andreas Opitz[1], Antje Vollmer[4], Wolfgang Brütting[3], Antoine Kahn[2], and Norbert Koch[1,4] — [1]Humboldt-Universität zu Berlin, Institut für Physik, Brook-Taylor-Str. 15, D-12489 Berlin, Germany — [2]Department of Electrical Engineering, Princeton University, Princeton, NJ 08544, USA — [3]Universität Augsburg, Institut für Physik, Universitätsstr. 1, D-86135 Berlin, Germany — [4]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH BESSY II, Albert-Einstein-Str. 15, D-12489 Berlin, Germany

We have used ultraviolet and inverse photoemission spectroscopy to determine the transport gaps (E_T) of C60 and diindenoperylene (DIP), and the photovoltaic gap (E_{PVG}) of five prototypical donor/acceptor interfaces used in organic photovoltaic cells (OPVCs). The transport gap of C60 (2.5 ± 0.1) eV and DIP (2.55 ± 0.1) eV at the interface is the same as in pristine films. We find nearly the same energy loss of ca. 0.5 eV for all material pairs when comparing the open circuit voltage measured for corresponding OPVCs and E_{PVG}.

DS 10.2 Mon 17:30 H32

Direct Observation of Charge Separation in Perylene Monoimide Solid State Dye-Sensitized Solar Cells — •Ian Howard[1], Michael Meister[1], Björn Baumeier[1], Henrike Wonnenberger[1], Neil Pschirer[2], Rüdiger Sens[2], Ingmar Brüder[2], Klaus Müllen[1], Denis Andrienko[1], and Frédéric Laquai[1] — [1]Max Planck Institute for Polymer Research, Ackermannweg 10, D-55128 Mainz, Germany — [2]BASF SE

Combining Vis-NIR broadband pump-probe transient absorption spectroscopy with precise measurement of the time-resolved photoinduced Stark effect we demonstrate that it is possible to track not only the rate of charge injection but also the motion of carriers after injection on the critical nanosecond timescale in Solid State Dye Sensitized Solar Cells. In terms of solar cell efficiency our findings have two major impacts. Firstly, we directly observe that the *reductive quenching* pathway previously suggested (wherein a photoexcited dye donates a hole to the hole transport material before then injecting an electron, now from the dye anion state, into the TiO2) is important for obtaining high device efficiencies, especially for NIR absorbing dyes which exhibit a reduced driving force for electron injection directly from the dye exciton. Secondly, we find that many charges return to the interface after following injection, likely due to Coulombic and image charge effects. Screening the charges better, for example by reducing the dielectric contrast or increasing the dye length, should decrease the interfacial charge density and thereby parasitic recombination.

DS 10.3 Mon 17:45 H32

Full electronic structure across a polymer heterojunction solar cell: interface dipoles and influence of light — •Johannes Frisch[1], Patrick Amsalem[1], Jens Niederhausen[1], Marcel Schubert[2], Eduard Preis[3], Antje Vollmer[4], Jürgen P. Rabe[1], Ullrich Scherf[3], Dieter Neher[2], and Norbert Koch[1] — [1]Humboldt-Universität zu Berlin, Germany — [2]Universität Potsdam, Germany — [3]Bergische Universität Wuppertal, Germany — [4]Helmholtz-Zentrum Berlin für Materialien und Energie - Speicherring BESSY II, Berlin, Germany

Controversial discussions concern the dependence of open circuit voltage on the energy offset between the highest occupied molecular orbital level of the donor material and the lowest unoccupied molecular orbital level of the acceptor material in organic photovoltaic cells. Therefore, we investigate the energy level alignment in two bilayer OPVCs comprising the donor poly(3-hexylthiophene) (P3HT) and the acceptors 1-(3-methoxycarbonyl)propyl-1-phenyl[6.6]C61 (PCBM) and poly(9,9'dialklylfluorene-alt- 4,7-bis(2,5-thiendiyl)-2,1,3-benzothiadiazole) (PFTBTT). Ultraviolet photoelectron spectroscopy revealed that notable interface dipoles occur at all interfaces across the OPVC structures for both material combinations. Particularly, the effective electrode work function (after contact formation with the organic material) differs significantly from those of the pristine materials. In addition, we find that negative charges are collected at the metal clusters (that exist in the early stage of cathode formation) due to exciton dissociation at the heterojunction.

DS 10.4 Mon 18:00 H32

Optoelectronic Properties Of Zinc(II)-Phthalocyanine — •Michael Kozlik, Sören Paulke, Marco Gruenewald, Roman Forker, and Torsten Fritz — University of Jena, Institute of Solid State Physics, Helmholtzweg 5, 07743 Jena, Germany

Zinc phthalocyanine (ZnPc) is an organic molecule which is used in organic optoelectronic devices, such as OLEDs and organic solar cells. Bulk material is represented mainly in form of the metastable α-ZnPc, while the stable β-ZnPc is less conductive [1]. We show the critical transformation temperature as well as optical and morphological differences between both phases. Description and simulation of the performance of organic devices make use of material parameters. In our work we present the determination of the optical constants and the exciton diffusion length. Experimental methods are UV-Vis spectroscopy and external quantum efficiency. By transmittance and reflectance spectra we derive the real and imaginary part of the refractive index [2]. In combination with the derived parameters we show the performance of a simplified photovoltaic cell and identify the region of exciton dissociation and exciton diffusion length.

References

[1] K. Wihksne et al., J. Chem. Phys. 34 (1961) 2184.
[2] M. Kozlik et al., Org. Electron. 13 (2012) 3291.

DS 10.5 Mon 18:15 H32

The operational mechanism of ionic transition metal complex-based light-emitting electrochemical cells — •Sebastian B. Meier[1,2], Stephan van Reenen[3], Henk J. Bolink[4], Martijn Kemerink[3], Wiebke Sarfert[2], and Albrecht Winnacker[1] — [1]Department of Materials Science VI: Materials for Electronics and Energy Technology, University of Erlangen-Nuremberg, Germany — [2]Siemens AG, Corporate Technology, CT RTC MAT MPV-DE, Erlangen, Germany — [3]Department of Applied Physics, Eindhoven University of Technology, The Netherlands — [4]Instituto de Ciencia Molecular, Universidad de Valencia, Spain

Light-emitting electrochemical cells (LECs) are promising candidates for cost-efficient next generation solid-state lighting and signage applications. They feature only a single, solution-processible active layer comprising a luminescent material in an ionic environment which allows for charge carrier injection from air-stable electrodes and low operating voltages. The operational mechanism of LECs has been the subject of an intense debate ever since their discovery. Evidence for electrochemical doping has been demonstrated for polymer-based devices, whereas LECs comprising ionic transition metal complexes (iTMCs) have almost exclusively been stated to operate via an electrodynamic mechanism. We used fluorescence as well as scanning Kelvin probe microscopy on planar iTMC-LECs to elucidate their mechanism of work. Our results illustrate profound evidence for electrochemical doping in these kind of LEC devices and highlight that the position of the established p-i-n junction is not fixed but migrates during device operation.

DS 10.6 Mon 18:30 H32

Effective Charge Carrier Lifetimes in Organic Solar Cells Prepared by Coevaporation of $C60$ and $CuPc$ in different mixtures and geometries — •André Dragässer and Derck Schlettwein — Institute of Applied Physics, Justus-Liebig-University Giessen, Giessen, Germany

Evaporated organic solar cells can lead to efficiencies of technical relevance if the interface of donor and acceptor molecules is optimized for the interplay of exciton dissociation, charge transport and recombination. The effective lifetime of the charge separated state is of central relevance. Intensity- modulated photovoltage spectroscopy with parallel impedance spectroscopy is a suitable method of analysis. Organic solar cells consisting of the well-established semiconductor materials $CuPc$ and $C60$ were prepared by physical vapor deposition on an ITO substrate, modified with $PEDOT : PSS$. The cells were completed by a back contact of BCP as a buffer and aluminum. Cell architectures of planar junctions, bulk heterojunctions or planar-mixed heterojunctions were studied for different film thickness of the components. IV-measurements in the dark and under varied illumination intensities provided basic device characteristics. Detailed measurements of the short-circuit photocurrent and the open-circuit photovoltage under static or intensity-modulated illumination with different wavelength were performed to determine the average charge carrier lifetime in the devices which was related to the respective charge carrier density obtained by impedance spectroscopy. Recombination reactions and, in particular, the influence of trap states will be discussed.

DS 11: Poster Session I: Application of thin films; Ion beam induced surface patterns; Ion and electron beam induced processes; Micro- and nanopatterning (jointly with O)

Time: Monday 17:00–20:00 Location: Poster B1

DS 11.1 Mon 17:00 Poster B1

Optical and structural properties of $ZnCo_2O_4$ under different growth conditions — •Vitaly Zviagin, Tammo Böntgen, Rüdiger Schmidt-Grund, Michael Lorenz, and Marius Grundmann — Universität Leipzig, Institut für Experimentelle Physik II, Linnéstr. 5, Germany

We present an investigation of optical and structural properties of $ZnCo_2O_4$ thin films in dependence on the growth conditions. The films were grown on an a-sapphire substrate by pulsed layer deposition at different oxygen partial pressures. The optical properties were determined by spectroscopic ellipsometry (SE) in the range from 0.5 eV to 9.0 eV. A model was developed for the measured dielectric function (DF) of the $ZnCo_2O_4$. Our model consists of Gauss- and critical-point-functions located at the optical transition energies. Transmission measurements in the same spectral range were carried out and reveal weak absorption bands below the band gap. The positions of the bands correspond to d-d transition of Co^{2+} known to arise in $ZnCo_2O_4$[1]. The thickness of the thin films and surface topology, estimated from atomic force microscopy and scanning electron microscopy, are comparable to the SE estimations. The crystal structure of the films was determined from the wide-angle X-ray diffraction scans which are presented and compared in dependence on the oxygen partial pressure of the film deposition. It was determined that the partial pressure during the deposition induces a distinct shift in the observed transition energies as well as clear dependence in the crystallography and surface topology of the thin films. [1] Wang et al., J. Alloys Compd. 520 (2012) 158.

DS 11.2 Mon 17:00 Poster B1

Controlling sputter yield during multilayer preparation for high resolution multilayer zone plates — •Christian Eberl[1], Florian Döring[1], Tobias Liese[1], Felix Schlenkrich[1], Volker Radisch[1], Hans-Ulrich Krebs[1], Anna-Lena Robisch[2], Aike Ruhland[2], Markus Osterhoff[2], Sarah Hoffmann[2], Matthias Bartels[2], and Tim Salditt[2] — [1]Institut für Materialphysik, University of Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany — [2]Institut für Röntgenphysik, University of Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

Due to the deposition of energetic particles, pulsed laser deposition (PLD) is a suitable technique to produce high-quality multilayers without cumulative roughness. Even surface roughness of a wire, on which aperiodic multilayers were grown for multilayer zone plates (MZP), could be smoothed. Unfortunately, the transferred energetic ions induce resputtering of deposited material, especially on such curved surfaces. Not loosing layer thickness or interface quality, both a fundamental understanding and controlling of the underlying processes are essential. For this purpose, the interface behaviours of very different materials, such as W and Si, have been investigated. In this context, resputtering of W (up to 2 nm) was observed by both in-situ deposition rate monitoring and x-ray reflectivity measurements and could be verified by dynamical simulations. This effect could successfully be controlled by adjusting the laser fluence for both Si and W. With this knowledge, a highly precise MPZ could be fabricated showing hard x-ray focusing with focal width of less than 10 nm (FWHM).

DS 11.3 Mon 17:00 Poster B1

Nanostructured TiO_2 thin films and structural composites for photocatalysis — •Bodo Henkel, Sebastian Zabel, Thomas Strunskus, and Franz Faupel — Institute for Materials Science, Kiel, Germany

Pulsed DC Magnetron Sputtering and various temperature treatments were used to produce improved photocatalytically active TiO_2 layers on quartz glass. Two approaches were used to improve decomposition of the test substance methylene blue. First, a structured liquid-diffusion open surface for larger interaction area was produced. At second, a synergetic multilayer combining the advantages of different TiO_2 structures was manufactured. This combination of different layers provides new insight on how the functional unit should be optimized to take into account the different physical processes important for photocatalysis. For measuring photocatalytic efficiency, decomposition of methylene blue in combination with in situ UV-vis measurement was used. An UV LED with 369 nm wavelength was taken to irradiate the TiO_2 layer. To analyze the correlation of dye decomposition rate to surface and crystal structure SEM, XRD, UV-vis and Raman spectroscopy measurements have been done.

DS 11.4 Mon 17:00 Poster B1

Turning graphene into the world's thinnest heater (It's nearly invisible!) — •Siamak Nakhaie, Stefanie Unseld, Jules Dake, and Carl Krill — Institute of Micro and Nanomaterials, Ulm University, Germany

The recent discovery of graphene and characterization of its extraordinary properties have ignited a firestorm of activity across the scientific community and corporate research world — many believe that graphene represents the basis for the smallest, fastest possible transistor. Of the various production methods currently under investigation, chemical vapor deposition (CVD) appears to be the most feasible for the large-scale production of graphene, and the number of CVD recipes that exist in the literature for single-layer graphene is nearly equal to the number of publications on the subject. We have systematically varied the various CVD process parameters, including temperature, pressure, gas flow rates and concentrations. In doing so, we were able to obtain amorphous, nanocrystalline, multi-layer or single-layer graphene samples. We also demonstrate how graphene can be used as a large-area, transparent electrode. By applying an electric current to our samples under ambient conditions, we were able to heat one square centimeter of single-layer graphene, supported on a glass substrate, to over 220°C.

DS 11.5 Mon 17:00 Poster B1

Nanosecond time-resolved temperature measurements — •Johann Berres, Elke Scheer, Paul Leiderer, and Johannes Boneberg — Department of Physics, University of Konstanz, Germany

Temperature evolution is studied in a thin silicon film after heating with a ns-laser pulse. For that purpose the reflectivity of a cw-laser is measured. Due to changes of the dielectric constants with temperature the interference conditions in the thin silicon film and thus the reflectivity vary, which allows the determination of the temperature with ns time-resolution. The measurements are compared with heat flow simulations. Finally examples for temperature evolution in samples which are illuminated by an interference pattern are shown.

DS 11.6 Mon 17:00 Poster B1

Immobilization of Gold Nanoparticles on Polyethylene glycol brushes for SERS sensing applications — •Claudine Dawson[1], Petra Uhlmann[1], Dieter Fischer[1], Guido Wilke[2], and Manfred Stamm[1,3] — [1]Leibniz-Institut für Polymerforschung Dresden e.V., Dresden, Germany — [2]Hochschule Esslingen, University of Applied Sciences, Esslingen, Germany — [3]Technische Universität Dresden, Dresden, Germany

Recent studies demonstrated that polymer brushes can be exploited for the formation of nanoassemblies with metallic nanoparticles for SERS applications1,2. Multifunctional polymer brushes offer multiple binding sites on which metallic nanoparticles can either be reduced in situ1 or preformed nanoparticles can be bound covalently2, coordinatively3 or electrostatically4 by tuning their surface chemistry. We demonstrate how coordinative binding of gold nanoparticles to polyethylene glycol brushes grafted on silica substrates can be used to control the immobilized amount and distribution of the particles by variation of the polymer grafting density and -chain length. Additionally the size of the bound gold nanoparticles was varied. The influence of these parameters on the signal enhancement in SERS was probed by using the dye Rhodamine 6G and correlated to the gold nanoparticle arrangement in the nanoassemblies which was investigated by scanning electron microscopy and atomic force microscopy.

1. Adv. Funct. Mater. 2010, 20, 1756*1761 2. J. Mater. Chem. 2012, 22, 5155*5163 3. ACS Nano 2009, 3, 807-818 4. J. Am. Chem. Soc. 2004, 126, 15950-15951

DS 11.7 Mon 17:00 Poster B1

Measurement of magnetoresistance effects in nanoscale metallic conductors — •Tobias Warnatz, Sebastian Wintz, Rantej Bali, Ulrich Wiesenhütter, Jochen Grebing, Jürgen Lindner, Jürgen Fassbender, and Artur Erbe — Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany

The magnetic characterization of nanoscale magnetic structures is one of the main prerequisites for the development of magnetoelectric memories and sensors. Here we present magnetoresistance effects of nanostructured metallic films and particles, which can exhibit anisotropic magnetoresistance or giant magnetoresistance effects. The structures are built from a variety of materials and they are measured at low temperatures in magnetic fields up to 1.5 T. We correlate the microscopic structure of the materials with the observed magnetic properties. Thus, a deeper understanding of switching and storage of the magnetic state in such nanostructures can be gained.

DS 11.8 Mon 17:00 Poster B1

Generating ultrashort circularly polarized XUV pulses from gas high harmonics by means of a multilayer quarter-waveplate — •Jürgen Schmidt[1], Alexander Guggenmos[2], Niklas Mutz[1], and Ulf Kleineberg[1,2] — [1]LMU München, Physik, 85748 Garching — [2]Max-Planck-Institut für Quantenoptik, 85748 Garching

Coherent linearly polarized XUV pulses from High Harmonic Generation in noble gas are routinely used for ultrafast pump-probe experiments to examine electron dynamics in solids or gases. The availability of circularly polarized high harmonic pulses with selectable helicity would extend the possible spectroscopic methods applicable to those pulses towards electron spin dependant or circular dichroism experiments and would give access to the investigation of temporal electron spin dynamics on a time scale of 1 fsec or even below. However, current concepts which aim at generating ultrashort elliptically polarized pulses from gas harmonics directly promise only a small ellipticity. We thus designed, fabricated and tested ultrathin multilayer-based quarter wave retarders at a photon energy of 66.2eV (Ni-3p state) to transform linearly polarized XUV pulses into circularly polarizd pulses . We investigate the polarization state of the pulses and the transmission characteristics of the quarter waveplate by means of a Rabinovich-type polarimeter with a multilayer analyzer mirror and an XUV spectrometer. A trade-off between pulse duration (i.e bandwidth) and degree of ellipticity is discussed and future experimental application in time-resolved ARPES experiments is described.

DS 11.9 Mon 17:00 Poster B1

Ion beam patterning of Si(001): from the amorphous to the crystalline regime — •Martin Engler, Moritz Will, and Thomas Michely — II. Physikalisches Institut, Universität zu Köln

It is well known that under room temperature irradiation Si ion beam amorphizes, while it remains crystalline during ion exposure at about 500 °C and above. In the present work we tune temperature through the amorphous-crystalline phase transition and investigate the effect of this transition on ion beam induced pattern formation. Scanning tunnelling microscopy and low energy electron diffraction are used to investigate the Si(001) morphology after 2 keV Kr$^+$ ion irradiation. With increasing temperature a sharp transition from a flat amorphous surface to crystalline mound and crater morphology is observed. The crystalline pattern displays a step and terrace structure with Si-dimer rows. The amplitude of the evolving crystalline pattern is highest right at the phase transition and decreases with increasing temperature within the crystalline regime. The opposite is true for the the lateral length scale of the pattern.

DS 11.10 Mon 17:00 Poster B1

On the origin of surface ripple propagation — •Hans Hofsäss, Kun Zhang, Omar Bobes, and Hans-Gregor Gehrke — II. Physikalisches Institut, U(niversität Göttingen, Germany

The Bradley-Harper theory predicts a lateral propagation of ripples in direction opposite to the incident ion beam dirdction [1]. However, a small or negligible ripple velocity was predicted [2,3]. Aat large incidence angles the propagation velocity should become large and positive, i.e. propagation along the beam direction. Several studies with Ga focused ion beams revealed ripple propagation at high velocities (+0.4 - +0.8 nm per 10Î5 ions/cm2) also for small incidence angles <65°, and a model able to explain the correct direction and magnitude of ripple propagation was proposed [4]. Wei et al. explained the positive propagation velocity by angle dependent sputtering of asymmetric ripple profiles [5]. We propose an additional mechanism for positive ripple propagation velocities based on ion-induced mass transport. We have measured the ripple propagation velocity for 10 keV Xe on Si and find a velocity of +3 nm per 10Î5 ions/cm2̂ at 70° incidence angle.

[1] R. M. Bradley and J. M. E. Harper, J. Vac. Sci. Technol. A 6, 2390 (1988).
[2] G. Carter, V. Vishnyakov, Phys. Rev. B 54, 17647 (1996).
[3] G. Carter, V. Vishnyakov, M.J. Nobes, Nucl. Instr. Meth. B 115 (1996) 440.
[4] P.F.A. Alkemade, Phys. Rev. Lett. 96, 107602 (2006).
[5] Q. Wei, J. Lian, L. Boatner, L.M. Wang, R.C. Ewing, Phys. Rev. B 80, 085413 (2009).

DS 11.11 Mon 17:00 Poster B1

Designing Si surface nanopatterns by low energy ion beams with metal surfactant sputtering — •Kun Zhang, Omar Bobes, and Hans Hofsäss — II. Physikalisches Institut, Universität Göttingen, Germany

Low energy ion sputtering can produce large area periodic self-organized surface nanostructures with potential applications. Recently we have demonstrated that metallic surfactants induce pronounced dot and ripple patterns on Si substrates during normal ion incidence sputter erosion. In the absence of metal co-deposition, uniform flat surfaces are obtained. We have shown that the produced surface nano-patterns strongly depend on the ion fluence and the deposition ratio, and their wave vectors are always parallel to the deposition direction. Based on these achievements, we further develop in this work the surfactant sputtering technique to produce self-organized surface nanostructures on Si with well defined symmetry, such as 4-fold, 5-fold or 6-fold symmetric dot nano patterns. In our experiments Si substrates were irradiated with 1 keV Ar ions at normal incidence and ion fluences up to 2.5x101̂8 ions /cm2̂ under continuous deposition of Fe atoms coming from a few Fe sputtering targets around the Si substrates with a certain geometrical arrangement.

DS 11.12 Mon 17:00 Poster B1

Ion beam enhanced etching of $LiNbO_3$ containing silver nano clusters for plasmonic waveguide applications — •Felix Felgenträger, Jura Rensberg, Steffen Milz, Carsten Ronning, and Werner Wesch — Institute of Solid State Physics, Friedrich Schiller University Jena

Plasmonic structures, consisting of nanometer sized metal clusters embedded in dielectric host materials, have been in the point of interest for the last two decades, due to their wide range of possible applications, like sensing, fast information transfer and the confinement of light. One of the most promising combinations for new plasmonic devices is lithium nobiate ($LiNbO_3$) as host material and incorporated noble metal nano clusters i.e. silver because of its distinct surface plasmon resonance in the visible range. In this contribution $LiNbO_3$ was implanted with a high amount of Ag^+ ions to form embedded Ag clusters. In situ as well as post implantation annealing was carried out to reduce radiation damage and recover the structure of the host material due to the preferential etching of amorphous $LiNbO_3$ with HF during waveguide fabrication. Argon ions were implanted selectively through a mask of photoresist prepared by standard photolithography for the ion beam enhanced etching step. Consequently μm-seized waveguide structures are formed by the unirradiated parts after etching. Cross-sectional STEM investigations were made in order to determine the waveguide structure and cluster size distribution. The optical properties of the Ag clusters were examined by the means of polarization-dependent UV-VIS absorption spectroscopy.

DS 11.13 Mon 17:00 Poster B1

Comparison of low- and room-temperature damage formation in Ar ion implanted GaN and ZnO — •E. Wendler[1], W. Wesch[1], A. Yu. Azarov[2], N. Catarino[3], A. Redondo-Cubero[3], E. Alves[3], and K. Lorenz[3] — [1]Friedrich-Schiller-Universität Jena, Institut für Festkörperphysik, Max-Wien-Platz 1, D-07743 Jena, Germany — [2]University of Oslo, The Department of Physics, P.O. Box 1048 Blindern, NO-0316 Oslo, Norway — [3]IST/ITN - Instituto Tecnológico e Nuclear, Instituto Superior Técnico,Universidade Técnica de Lisboa. Estrada Nacional 10, P-2686-953 Sacavém, Portugal

GaN and ZnO are implanted at 15 K and 295 K with 300/200 keV Ar ions. Damage analysis is performed with RBS in channelling configuration quasi-insitu at the respective temperature. The difference in minimum yield is taken as a measure of the amount of damage produced. The most striking result of our work is that in GaN and ZnO the ion-induced damage formation is only weakly influenced by the implantation temperature. For the discussion of our findings, results on damage formation in these materials obtained by other authors applying TEM are taken into account. Eventually it can be concluded that in these materials extended defects form not only at room temperature but also at a temperature of 15 K. This clearly suggests that the formation of extended defects is not driven by the thermal mobility of point defects. It is supposed that in GaN and ZnO damage-induced strain plays a dominant role and the formation of extended defects seems to be energetically favourable in comparison to the formation of larger randomly ordered agglomerates of defects.

DS 11.14 Mon 17:00 Poster B1

Binary Pt-Si nanostructures prepared by focused electron-beam-induced deposition: Simulation and experiment — •Marcel Winhold[1], Christian H. Schwalb[1], Fabrizio Porrati[1], Roland Sachser[1], Kaliappan Muthukumar[2], Harald O. Jeschke[2], Roser Valenti[2], and Michael Huth[1] — [1]Physikalisches Institut, Goethe-Universität, Max-von-Laue-Str.1, 60438 Frankfurt am Main — [2]Institut für Theoretische Physik, Goethe-Universität, Max-von-Laue Str. 1, 60438 Frankfurt am Main

Binary systems of Pt-Si were prepared by focused electron-beam-induced deposition (FEBID) using the two precursors $MeCpPt(Me)_3$ and $Si(SiH_3)_4$ simultaneously. This new approach for the preparation of binary systems with FEBID allows for the variation of the relative flux of the two precursors during deposition. The composites which contain Pt, Si, C and O in different ratios were analyzed by means of energy dispersive X-ray spectroscopy, atomic force microscopy, electrical transport measurements, and transmission electron microscopy. The results show strong evidence for the formation of an amorphous, metastable Pt_2Si_3 phase, leading to a maximum of the conductivity for a Si:Pt ratio of 3:2.[1] For the stoichiometric proportion of Si:Pt = 3:2 theoretical simulations applying an evolutionary algorithm (USPEX) predict the formation of Pt_2Si_3 layers separated by graphene-like planes. Micro-Raman measurements will be presented to experimentally study the Pt, Si, C and O structural configuration.

[1] Winhold et al., ACS Nano, 2011, 5 (12), pp 9675-9681

DS 11.15 Mon 17:00 Poster B1

Influence of electron beam parameters on the composition and conductivity of deposits prepared via focused electron-beam-induced deposition — •Paul M. Weirich, Marcel Winhold, Christian H. Schwalb, and Michael Huth — Physikalisches Institut, Goethe-Universität, Max-von-Laue-Str.1, 60438 Frankfurt am Main

Focused electron-beam-induced deposition (FEBID) is a high resolution one-step technique, which allows producing micro- and nanostructures. In many cases it becomes necessary to prepare structures with a high metal content, e.g. for contacting nanowires which for many precursors strongly depends on the deposition parameters. For the precursor tungsten hexacarbonyl $W(CO)_6$ it has already been shown, that the metal content of the deposits can be tuned by changing the electron beam parameters acceleration voltage and beam current [1]. Based on those experiments we further investigated the influence of the scanning parameters of the electron-beam - dwell-time and pitch - on conductivity and metal content of the tungsten deposits. The deposits were analyzed by means of in-situ electrical conductivity measurements, energy dispersive X-ray spectroscopy, atomic force microscopy and electrical transport measurements. The results show that by choosing the ideal combination of scanning parameters the metal content of the deposits can be raised from 25 at% up to 40 at% which leads to an increase of conductivity by almost two orders of magnitude.

[1] F. Porrati, R. Sachser and M. Huth, Nanotechnology 2009, 20, 195301

DS 11.16 Mon 17:00 Poster B1

Submicrometer precise machining of metal surfaces with excimer laser radiation — •Martin Ehrhardt, Frank Frost, Pierre Lorenz, and Klaus Zimmer — Leibniz-Institut für Oberflächenmodifizierung e. V., Permoserstraße 15, 04318 Leipzig, Germany

In recent decades, the patterning of surfaces with nanostructures is of rapid growing interest due to the large range of applications of these improved surfaces in the fields of, e.g. optics, biology, and microelectromechanical systems. Imprint techniques are promising for low-cost and large-area pattering. However, imprint techniques which allow submicrometer structuring of hard materials like metals have to be combined with an etching step up to now. Laser embossing is a novel high strain rate imprint technique which allows overcoming this limitation. The process bases on laser pulses which generate a high pressure by ablation of an auxiliary material. The high pressure is used to compress a structured mould form onto metal surfaces which take the shape of the mould. In the present study it will be shown that submicrometer structures can be successfully transferred from the mould into polycrystalline and single crystal copper. The structures generated that way will be analyzed by scanning electron microscopy (SEM) and atomic force microscopy (AFM). The results will be correlated with the laser parameters used and the dimensions of the mould structures.

DS 11.17 Mon 17:00 Poster B1

Molecule aggregate position control on patterned surface — •Wenchong Wang, Hong Wang, Harald Fuchs, and Lifeng chi — Physikalisches Insitut, Westfälische-Universität Münster, Wilhelm-klemm-Str. 10, 48149 Münster, Germany

Small molecular weight organic molecules are of great interest owing to their intensive applications. However, techniques for producing organic patterns, like photolithography in inorganic semiconductors, is still urgently sought for in device processing.

Considering a molecule deposited on a substrate surface at elevated temperature, the molecule could nucleate either at defect locations, step edges or aggregate together to form a stale nuclei. Previously, we have demonstrated to grow molecules on the pre-defined *defects* and *step edges* by using template induced growth strategies. However, molecule aggregate position control is extremely difficult owing to the statistic diffusion process of molecule on surface. Here we present a way to create molecule density distribution over a limited surface. The molecules nucleate initially at locations with highest density, leading to an aggregate position control.

Reference:
1. W. C. Wang, and L. F. Chi, Acc. Chem. Res., 2012, 45, 1646.
2. W. C. Wang, L. F. Chi, et al, Small, 2011, 7, 1403.
3. W. C. Wang, L. F. Chi, et al, Adv. Mat. 2010, 22, 2764.
4. W. C. Wang, L. F. Chi, et al, Adv. Mat. 2009, 21, 4721.
5. W. C. Wang, L. F. Chi, et al, Phys. Rev. Lett., 2007, 98, 225504.

DS 11.18 Mon 17:00 Poster B1

Optimization and characterization of liquid metal ion sources for focused ion beam technology — •Alexander Schwinger, Rüdiger Schott, and Andreas D. Wieck — Lehrstuhl für angewandte Festkörperphysik, Ruhr-Universität Bochum

Focused ion beam devices are widely used for maskless ion implantation and milling on a nanometer scale. In order to increase the performance and stability of liquid metal ion sources (LMIS) commonly used in focused ion beam (FIB) systems, we produced and compared multiple needle type LMIS. Preparation of tip and surface of the LMIS was done by gradual electrochemical etching of tungsten wire, the resulting surface topology and tip geometry were investigated with SEM. After filling the LMIS with the source material, the dependency of the emitted ion current on the extraction voltage was measured. Long-term emission stability was then evaluated by measuring the variation of the ion current over time while applying a constant extraction voltage.

DS 11.19 Mon 17:00 Poster B1

Fabrication, characterisation and optimization of liquid alloy ion sources for nano structuring and lithography — •Michael Kwiatek[1], Rüdiger Schott[1], Paul Mazarov[2], and Andreas D. Wieck[1] — [1]Ruhr-Universität Bochum — [2]Raith GmbH, Dortmund

Focussed Ion Beam (FIB) and ion lithography systems are tools gaining more attention in R&D and industrial applications. The source material mostly used in those systems is Gallium (Ga). But for common applications one need other implantation materials like Silicon (Si) or Gold (Au) that are electrical interesting and for some applications important - bio compatible. Furthermore materials with a low atomic weight (a.w.) are interesting for less destructive and sharper imaging with the FIB column. So there started a trend to non-Ga-FIBs in the past few years. Our solution to this problem are Liquid Alloy Ion Sources (LAIS) containing not only one but 2 to 3 different materials in one alloy which's composition is picked in an eutectic point for a relative low melting point. Those sources require a mass filter in the beam column but the new possibilities outweight that as you have an emission stable source that contains e.g. a good sputtering material (high a.w.) and a good imaging material (low a.w.) that can be used without changing the source. This brings a field of new possibilities and usages. We optimized an AuSiLi and an AuSiBe ternary source for sputtering-implanting-imaging purpose to get in the emission stability regions of pure Ga sources.

DS 11.20 Mon 17:00 Poster B1

Nanolithography using Electron Field Emission from Nanotips — •Steve Lenk, Marcus Kästner, Tzvetan Ivanow, and Ivo Rangelow — Institut für Mikro- und Nanoelektronik, Technische Universität Ilmenau, Germany

The emission of low-energetic electrons from a scanning probe nanotip is a promising method to produce nanometer-scale semiconductor devices [1]. We study the electron emission from metallic and semiconducting nanotips with regards to the application in nanolithography experimentally and theoretically. The operation regime for the electron lithography, i.e. applied voltages up to 50V and operation at room temperature, is between field and thermionic emission. In addition to the calculation of the field emission current, we are solving Laplace's equation for the electric field distribution around the nanotip and the trajectories of the emitted electrons. To achieve an additional focusing of the electron beam, we include a volcano-type gate [2]. In nanolithography applications semiconductor tips are often used and, therefore, we consider the effects of field-induced changes of band bending, surface charges as well as the effect of screened image charges and emission from surface states together with a volcano gate. The theoretical results were compared with Fowler-Nordheim measurements. These measurements and calculations are the basis for study the interactions of the emitted electrons with the resist material and, thus, to the mechanisms of nanolithography.

[1] M. Kaestner and I. Rangelow, Microelectron. Eng. 97 (2012) 96
[2] T. Ivanov, J. Vac. Sci. Technol. B 19 (2001) 2789

DS 11.21 Mon 17:00 Poster B1

Scanning Tunnelling Spectroscopy of FIB-induced Local Phase Changes in Tetrahedral Amorphous-Carbon — •Frederik Klein[1], Peter Philipp[2], Lothar Bischoff[2], and Thomas Mühl[1] — [1]Leibniz-Institut für Festkörper- und Werkstoffforschung Dresden — [2]Institut für Ionenstrahlphysik und Materialforschung, Helmholtz-Zentrum Dresden-Rossendorf

Ion irradiation of tetrahedral amorphous-carbon leads to both an ion implantation and a local phase change of the carbon. The latter is equivalent to an increase of the carbon sp2/sp3 bond ratio. It is caused by the deposition of the ion energy and leads to an increased electrical conductivity. We perform spatially resolved scanning tunneling spectroscopy in order to investigate the impact of different ion species (Ga, Si, Ge, Au). A direct contribution of the implanted metal will be carefully considered.

DS 11.22 Mon 17:00 Poster B1

Dewetting of silver films on Al-doped ZnO for plasmonic nanofilm formation — •Patrick Hofmann[1], Mykola Vinnichenko[2], Steffen Cornelius[2], Barbara Abendroth[1], Karl-Heinz Heinig[2], Sibylle Gemming[2], and Dirk-Carl Meyer[1] — [1]Institut für Experimentelle Physik, Leipziger Straße 23, 09599 Freiberg, Deutschland — [2]Institut für Ionenstrahlphysik, Helmholtz Zentrum Dresden Rossendorf, Bautzner Landstraße 400, 01328 Dresden, Deutschland

Up to now all thin film solar cells exhibit only low efficiency around 6 to 8 %. This low value stems mainly from their thin absorbing layer; hence light management is a real challenge. One possibility to increase light absorption is the development of scattering mechanisms for light, which nears the backside of the solar cell and leads to an effective increase of the light path in the absorber. This work presents an approach to the fabrication of plasmonic Ag-Nanoparticles in ZnO:Al matrices by dc magnetron sputtering and subsequent dewetting treatment. For this purpose, both vacuum annealing and millisecond high power diode laser processing were tested. The dewetting of Ag layers is investigated by scanning electron microscopy. Depending on the processing parameters, the morphologies ranging from percolated network of islands to completely dewetted films were obtained. Spectral photometry in transmission and reflection showed stronger plasmonic features for laser annealed Ag-AZO composite layers in comparison with thermal vacuum annealed samples. The plasmonic effects become more pronounced with increasing laser power density and dwell time.

DS 11.23 Mon 17:00 Poster B1

Continuous wave UV-laser sintering of ink-jet printed ZnO nanoparticle thin films at low laser powers — •Alice Sandmann[1], Jens Theis[2], Axel Lorke[2], Christian Notthoff[1], and Markus Winterer[1] — [1]Nanoparticle Process Technology and CeNIDE, Universität Duisburg-Essen, Lotharstr.1, 47057 Duisburg, Germany — [2]Fachbereich Physik and CeNIDE, Universität Duisburg-Essen, Lotharstr.1, 47057 Duisburg, Germany

We present continuous wave UV-laser sintering experiments of ZnO nanoparticle thin films prepared by ink-jet printing. The ZnO nanoparticles are printed on interdigital gold structures on quartz substrates and characterized by conductivity and microphotoluminescence measurements. The microstructure of the nanoparticle thin films is obtained by scanning electron microscopy. We show that laser sintering can be observed even at laser powers as low as 30 mW, using an UV-laser at 325 nm focused to a 10 μm spot. Furthermore, we describe the laser heating process numerically using an iterative finite element algorithm, which couples the heat equation with a simplified sintering model. The numerical and experimental results match well and reveal two key parameters responsible for the effective heating and sintering process: The laser wavelength in relation to the wavelength corresponding to the band gap of the material and the initial porosity of the film.

DS 12: Poster Session II: Functionalized semiconductor nanowires (jointly with HL); Resistive switching (jointly with DF, KR, HL); Thermoelectric materials

Time: Monday 17:00–20:00 Location: Poster B1

DS 12.1 Mon 17:00 Poster B1

Optical properties of Sn-doped CdS nanowires — •Marcel Wille[1], Sebastian Geburt[1], Robert Röder[1], Mengyao Zhang[2], Jia Grace Lu[2], and Carsten Ronning[1] — [1]Institut für Festkörperphysik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena — [2]Department of Physics and Electrical Engineering, University of Southern California, Los Angeles, USA

Nanowires (NWs) are promising candidates for future optoelectronic applications due to their possibility of light generation, waveguide properties and light amplification in a Fabry-Perot resonator. The controlled modification of their electrical and optical properties, for example by doping, will continue the consequent progress in NW research. The in-situ doping during the VLS synthesis is a difficult task due to the restricted solubility of dopants in gold (Au), which is typically used as catalyst. Therefore, we investigate an alternative catalyst (Sn) in order to succeed in successful doping during growth. SEM an TEM were performed to analyse the morphology of CdS NWs synthesized under usage of Sn as catalyst. The stoichiometry and successful doping with Sn was proven by EDX point measurements and mappings. In micro-PL, macro-PL and CL measurements at low and room temperatures the NBE, DLE and DAP (donor-acceptor pair) transitions were investigated to state about the optical properties. The occurring DAP transition, which was proven by power- and temperature dependent PL measurements, indicates the successful incorporation of Sn into the CdS NWs.

DS 12.2 Mon 17:00 Poster B1

Tailoring CdS nanowire lasing resonators — •Robert Röder[1], Sebastian Geburt[1], Andreas Johannes[1], Markus Glaser[2], Alois Lugstein[2], and Carsten Ronning[1] — [1]Institut für Festkörperphysik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, D-07743 Jena — [2]Institut für Festkörperelektronik, TU Wien, Floragasse 7, A-1040 Wien

The nanophotonics research for the development of on-chip optical components has to be intensified due to the forthcoming limits of conventional electronic integrated circuits. Semiconductor nanowires mark the physical size limit of a multimode photonic laser system. Thus, they are promising for circumventing these limits via optical data transmission and processing. The green spectral range around 2.4 eV is made accessible by high quality VLS synthesized cadmium sulfide nanowires (CdS NW) acting as Fabry-Pérot laser resonators with a remarkable low threshold of 10 kW/cm^2 at room temperature [Geburt et al, Nanotechnology 23, 365204 (2012)]. The resulting task for the processing of CdS nanolasers with reproducible properties remains in defining the resonator: The mode spacing can be adjusted by reducing the cavity length. The reflectivity of the guided modes can be enhanced as well by polishing the facet ends. Thus, preparation techniques for tailoring the resonator are demonstrated using focused ion beams (FIB) and a focused laser beam.

DS 12.3 Mon 17:00 Poster B1

Luminescence decay dynamics of colloidal CdSe quantum dots in different environments — •Michael Diez[1], Stephanie Bley[1], Dongchao Hou[1], Sebastian Resch[2], Siegfried Waldvogel[2], Jürgen Gutowski[1], and Tobias Voss[1] — [1]Institute of Solid State Physics, Semiconductor Optics, University of Bremen, 28359 Bremen, Germany — [2]Institute of Organic Chemistry, Johannes Gutenberg University Mainz, 55128 Mainz, Germany

The functionalization of semiconductor surfaces with colloidal quantum dots has gained substantial interest because of its wide application in optical sensing and energy harvesting. The quantum dots can be selectively attached to semiconductor surfaces with the help of linker molecules. We have studied the luminescence decay dynamics of colloidal CdSe quantum dots functionalized with ω-mercapto alkanoic acid in different environments. As optical excitation source we use a frequency-doubled Ti:sapphire laser ($\lambda = 350\,nm$, $\Delta t = 60\,fs$, $f = 82\,MHz$ and $E_{pulse} = 12\,nJ$). We detect the luminescence signal with a streak camera and an attached spectrometer ($\Delta t < 2\,ps$, $\Delta\lambda < 0.2\,nm$). For colloidal CdSe quantum dots in aqueous solution, we find that the luminsescence decay time can be well fitted with a biexponential decay (shorter decay time $t_1 \approx 200\,ps$, longer decay time $t_2 \approx 3\,ns$). Furthermore, we discuss the importance of surface and bulk states for the observed biexponential decay and study the change of t_1 and t_2 for quantum dots attached to different oxide surfaces. The observed results will allow for the optimization of quantum dot properties for specific optoelectronic applications.

DS 12.4 Mon 17:00 Poster B1

Einfluss der Prozessparameter auf das Wachstum von ZnO-Nanodrähten — •Matthias Ogrisek, Andreas Johannes und Carsten Ronning — Friedrich-Schiller-Universität, Jena, Deutschland

ZnO Nanostrukturen können sehr einfach über Gasphasentransport und -Abscheidung in einem horizontalen Rohrofen synthetisiert werden. In den vergangenen Jahren stand hier insbesondere die Herstellung von ZnO Nanodrähten über den Vapor-Liquid-Solid (VLS) Mechanismus im Fokus. Dabei ist das Verständnis über die wechselseitigen Einflüsse der einzelnen Prozessparameter auf die resultierenden Nanostrukturen nicht vollständig geklärt. ZnO Nanodrähte und andere Strukturen wurden durch thermisches Verdampfen von ZnO:C Pulver (carbothermal method) auf verschiedenen Substraten (SiO2, AZO) gewachsen. Die sich gegenseitig beeinflussenden Prozessparameter erlauben dabei das Wachstum von Nanodrähten bei sehr unterschiedlichen Bedingungen. Untersucht wurden die erzeugten ZnO Nanostrukturen mittels Rasterelektronenmikroskopie (REM) und Photolumineszenz-Spektroskopie (PL). Über den Vergleich der Bandkantennahen- und Defektbandemission lassen sich Rückschlüsse auf die relative Defektkonzentration ziehen.

DS 12.5 Mon 17:00 Poster B1

Growth of GaAs nanowires using the ANKA portable MBE system — •Jean-Wolfgang Hornung[1], Emmanouil Dimakis[2], Philipp Schroth[1], Lutz Geelhaar[2], and Tilo Baumbach[1] — [1]Karlsruhe Institute of Technology, Institute for Photon Science and Synchrotron Radiation, Karlsruhe, Germany — [2]Paul-Drude-Institut für Festkörperelektronik, Berlin, Germany

We present results on first growth experiments with the portable Molecular Beam Epitaxy (PMBE) System at ANKA performed at the PDI in Berlin. This system enables the growth of nanostructures in the (In,Ga)As-material system and in-situ monitoring of growth processes using synchrotron radiation at various synchrotron radiation facilities such as ANKA, ESRF, PETRA III. The properties of such NWs are of great importance for the fabrication of high performance electronic devices such as vertical transistors and solar cells.

For future time-resolved XRD-measurements on single NWs, the control of the axial growth rate and number density is very important. We show that by changing the growth parameters (growth temperature, V/III-ratio) we were able to influence these properties. In particular we grew self-catalyzed GaAs-Nanowires (NWs) on Si(111) substrates covered with thin oxide layers of different thicknesses. Insitu the growth process was monitored using RHEED measurements. Ex-situ the samples were characterized by SEM measurements.

We gratefully acknowledge the help of C. Hermann, A.-K. Bluhm and H. - P. Schönherr at PDI, as well as the support by Dr. B. Krause and H.-H. Gräfe at ANKA.

DS 12.6 Mon 17:00 Poster B1

Structural and resistive switching properties of SrTiO$_3$ deposited by RF sputtering — •Benjamin Roessler, Jura Rensberg, Frank Schmidl, and Carsten Ronning — Institut für Festkörperphysik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany

Strontium titanate (SrTiO$_3$) exhibits bipolar resistive switching between a high- and a low-resistance state when applying an appropriate electric field. The possibility to deposit SrTiO$_3$ at room temperature by magnetron sputtering on silicon substrates without buffer layers makes it one of the promising candidates for future nonvolatile data memory application. Therefore, we deposited polycrystalline SrTiO$_3$ on p-Si(100) as well as p-Si(110) at room temperature with a fixed oxygen-to argon content ratio of 1:2. The microstructure as well as the crystalline quality of the films was analyzed using cross-sectional electron microscopy and X-ray diffraction analysis. For both substrates a broad grain size distribution was found for the as-deposited films. To improve the crystalline quality post-deposition annealing was performed up to temperatures of 1000°C. In this contribution we discuss the structural changes and electrical properties of SrTiO$_3$, i.e. the resistive switching properties as a function of the annealing temperature.

DS 12.7 Mon 17:00 Poster B1

Memory Effects in Resistive Ion-beam Modified Oxides — •S. Gemming[1,2], D. Blaschke[1,2], K. Potzger[1], P. Zahn[1], A. Bogusz[2], H. Schmidt[2], T. Mikolajick[3], S. Slesazeck[3], H. Wylezich[3], B. Abendroth[4], D. C. Meyer[4], S. Rentrop[4], R. Dittmann[5], K. Skaja[5], R. Waser[5], J. Rensberg[6], C. Ronning[6], N. A. Spaldin[7], and D. Basov[8] — [1]HZ Dresden-Rossendorf, D-01314 Dresden — [2]TU Chemnitz, D-09107 Chemnitz — [3]TU Dresden, D-01062 Dresden — [4]TU Bergakademie Freiberg, D-09596 Freiberg — [5]FZ Jülich, D-52425 Jülich — [6]Friedrich Schiller University Jena, D-07743 Jena — [7]ETH Zürich, CH-8092 Zürich, Switzerland — [8]U.C. San Diego, La Jolla CA 92093-0354, U.S.A.

The Virtual Institute 'Memriox' establishes a joint research initiative in the field of ion-tailored oxide-based memristive elements, to be pursued within a novel and unique combination of core competences from the Helmholtz centers Dresden-Rossendorf and Jülich and their university partners in Dresden, Freiberg, Jena, San Diego, and Zürich. A nanoscale memristive element may prove the concept of the ultimate future non-volatile memory cell with a resistance set directly by electric currents. The Virtual Institute aims at stepping beyond the established layer-by-layer control of intrinsic defects during the synthesis of memristive homojunctions. The project is financed by the Initiative and Networking Funds of the Helmholtz Association (VH-VI-442).

DS 12.8 Mon 17:00 Poster B1

Transmission X-ray microscopy of resistively switched epitaxial Fe-doped SrTiO3 MIM structures — •Holger Wasmund[1], Annemarie Köhl[1], Peter Guttmann[2], Katja Henzler[2], Stephan Werner[2], Sebastian Schmelzer[1], Regina Dittmann[1], and Rainer Waser[1] — [1]FZ Jülich, PGI-7, Germany — [2]HZB, Institute for soft Matter and functional Materials, Germany

There exists strong experimental evidence that the resistance change in transition metal oxides is caused by a valency change on a nanoscale. Transmission X-ray microscopy exhibit the potential of observing bulk spectral information of the sample with a spatial resolution of 25nm unlike other methods which exclusively probe the surface e.g. XPS. One central issue in TXM probe preparation is the sample thickness which should not exceed 100nm. As a first approach we studied polycrystalline STO devices on SiN membranes which were switched in two different resistive states. To analyse epitaxial grown STO devices we prepared SRO|STO|Pt MIM structures on top of NGO substrates with an intermediate sacrifical layer by pulsed laser deposition and sputtered Pt electrodes. A chromium adhesion layer and a carbon film were deposited on top of the stack in order to serve as a carrier foil, followed by a selective etching step of the sarifical layer to release the specimen from the substrate. XAS spectra measurements at the Ti L edge and the Fe L edge for electrode pads in different resistive states were realized at the U41 beamline at Bessy II. We observed significant changes in the Ti spectra which are indications for a valency change in a filament like region.

DS 12.9 Mon 17:00 Poster B1

Adaptive Robot learning via (simulated) memresistive Elements — •Marius Schirmer and Andy Thomas — Bielefeld University, Bielefeld, Germany

Memristors are new circuit elements that fill the gap in relations between the circuit variables flux ϕ and charge q. Like their name consisting of *Mem*ory and Res*istor* presumes, they are resistors with memory. The resistance depends on the current *i(t)* that was applied to an element earlier. This behavior is similar to the synapse of a living nerve cell and therefore networks of memristors can be used as neuronal networks in hardware circuits.

To visualize the learning process of such a memresistive neuronal network we used a *Lego Mindstorms NXT* robot and designed an interface for using memristors that can be connected to the *NXT brick*. We also designed a circuit board that is simulating memresistive behavior. The Software written in Java allows several different learning tasks.

DS 12.10 Mon 17:00 Poster B1

Thermal conductivity measurements using the Raman shift method — •Simon Filser, Benedikt Stoib, Martin Stutzmann, and Martin S. Brandt — Walter Schottky Institut, Technische Universität München, Am Coulombwall 4, 85748 Garching

With the aim to determine the in-plane thermal conductivity of laser-sintered thin films of SiGe nanoparticles [1], we study the applicability of a contactless optical method employing the temperature-dependent frequency shift of the LO phonon mode, as observed by Raman spectroscopy, as a measure for the local temperature. We present our results on a variety of model systems such as, e.g., bulk Si, free-standing Si films and rectangular cantilevers validating the method. The pressure-dependent influence of parasitic thermal conduction through the ambient atmosphere is studied, indicating a small effect for single crystalline material, but a significant contribution for the macro-porous laser-sintered system studied here. Free-standing samples of laser-sintered Si nanoparticle thin films were fabricated either by scanning electron microscope-based micro-manipulation or via a liquid-transfer technique. The results of Raman mapping of such membranes are consistent with the sample morphology and provide insight into the thermal transport.

[1] B. Stoib et al., Appl. Phys. Lett., **100**, 231907 (2012)

DS 12.11 Mon 17:00 Poster B1

A real space method for third-order IFCs and phonon relaxation times for Si from first principles — •Marcel Giar, Michael Bachmann, and Christian Heiliger —)I. Physikalisches Institut, Justus-Liebig-Universität, D-35392 Giessen, Germany

We present a real space method to obtain third-order phonon anharmonicities from first principles calculations. The anharmonic interatomic force constants (IFCs) of third order are determined from a real space method involving small displacements of atoms inside a supercell. We calculate the anharmonic IFCs from force fields due to the displaced atoms using the Vienna *Ab Initio* Simulation Package (VASP). We determine the third-order anharmonicities of the potential for the case of silicon (Si). From these the phonon relaxation times for Si are obtained for different phonon branches.

DS 12.12 Mon 17:00 Poster B1

Phonon Transport in Si-Isotope-Multilayer — •Michael Bachmann, Michael Czerner, Robert Henrich, and Christian Heiliger — I. Physikalisches Institut, Justus Liebig University Giessen, D-35392, Germany

In thermoelectrics the maximum achievable efficiency is linked to the material parameters by the so called figure of merit. There are in principle four different material parameters, which can be divided into three electronic parameters and one phononic parameter. The three electronic parameters are the electric conductivity, the Seebeck coefficient, and the thermal conductivity of the electrons. The phononic parameter is the thermal conductivity of the lattice. In silicon the electronic parameters are suitable for thermoelectric applications, but the high lattice thermal conductivity prevents the application of pure silicon in thermoelectric devices. Si-isotope-multilayers are a promising structure, where the lattice thermal conductivity can be decreased and the electronic parameters remain unaffected. We present phonon transport calculations based on an atomistic Greens function method for ^{28}Si/^{29}Si and ^{28}Si/^{30}Si isotope-multilayers. These results show that a periodic arrangement of the layer-system cannot decrease the phonon thermal conductivity substantially, whereas a random arrangement of the layer-system can lead to a strong decrease in the phonon conductivity.

DS 12.13 Mon 17:00 Poster B1

Glancing Angle Deposited Silicon/Germanium Nanostructures for Electronic Applications — •Christoph Grüner and Bernd Rauschenbach — Leibniz-Institut für Oberflächenmodifizierung, Permoserstraße 15, D-04318 Leipzig, Germany

Obtaining control over the physical properties of semiconductors is a big challenge for future electronics. The use of nanostructures can provide this control, since quantum mechanical and surface effects become important. Nanostructured thin films can show higher optical absorption or reduced reflectivity, higher thermal resistivity and altered electrical properties compared to bulk material. Most preparation techniques for such structures, like etching or VLS growth, are limited by a small window of usable materials or process conditions. With Glancing Angle Deposition (GLAD) it is possible to produce nanostructures from a wide range of materials and with highly customizable shapes, such as slanted and vertical wires, spirals or zig-zag structures. In this technique a highly oblique incidence of deposited material causes small obstacles to cast shadows during the high vacuum deposition, so that areas behind them do not receive material. This leads to the growth of a highly porous thin film. The shape of the individual structures can be influenced by a controlled substrate rotation. We present silicon/germanium GLAD heterostructures with different shapes, a varying germanium distribution and adjustable doping. We also show some approaches to prepare electrical contacts to nanostructure arrays for device integration.

DS 12.14 Mon 17:00 Poster B1

Thermoelectric characterization of Sn$_1$(V)$_2$(VI)$_4$ substitutional systems — •Stefan Jakobs[1], Felix Rolf Lutz Lange[1], Karl Simon Siegert[1], Peter Jost[1], and Matthias Wuttig[1,2] — [1]I. Physikalisches Institut (IA), RWTH Aachen University, 52056 Aachen, Germany — [2]JARA - Fundamentals of Future Information Technology, RWTH Aachen University, Germany

The environmental impact of global warming and the steady rise of the world-wide energy demand requires an increased efficiency of energy consumptive applications.

Thermoelectric generators may contribute to increased efficiency since they are able to convert waste heat into electrical energy. The conversion efficiency of thermoelectric materials is characterized by the dimensionless figure of merit $zT = \frac{\alpha^2\sigma}{\kappa}T$. Hence, to gain large zT values, it is mandatory to have a high electrical conductivty σ, a large Seebeck coefficient α and a low thermal conductivity κ. Since charge carriers also contribute to thermal transport, low lattice thermal conductivities are crucial for a high thermoelectric performance.

Thin film (IV)$_1$(V)$_2$(VI)$_4$ chalcogenides allow access to a metastable rocksalt phase. While one sublattice consists of Te, the cation site is randomly occupied by Sn, Sb and 25% of vacancies. This unconventionally high degree of disorder in combination with the large amount of vacancies is favourable for low lattice thermal conductivities [1].

Here, we present the thermoelectric properties of Sn$_1$Sb$_2$Te$_4$ and Sn$_1$Bi$_2$Te$_4$ thin films prepared under different annealing conditions.
[1] E. R. Sittner *et al.*, *Phys Status Solidi* **A**, DOI 10.1002/pssa.201228397

DS 12.15 Mon 17:00 Poster B1

Transport through nano sized pillars — •Thorben Bartsch, Alina Wetzel, David Sonnenberg, Christian Heyn, and Wolfgang Hansen — Institut für Angewandte Physik und Zentrum für Mikrostrukturforschung, Jungiusstraße 11, 20355 Hamburg, Germany

We fabricate GaAs nanopillars with typical lengths between 4-8 nm and diameters of about 100 nm using molecular beam epitaxy [1]. The pillars are linked to a GaAs substrate on one end and to a GaAs layer of variable thickness at the other end. The epitaxial growth of the structure ensures that there are no crystal interfaces at these contacts. The pillars are embedded in a matrix of AlAs that can be selectively removed with hydrofluoric acid.

When the AlAs matrix is removed, the pillars open a gap between the GaAs layer and the substrate [1]. Appling a thermal gradient across the gap, thermal transport through the pillars can be studied. Using the 3-omega method we verified that the thermal transport through the pillars is ballistic in a temperature range at least up to 150 K [2]. Here influences from variations of the heterostructure geometry, especially from variable top layer thicknesses are discussed.

Moreover, in case of doped structures, charge transport through the pillars between two charge reservoirs held at different electric potential can be studied. We present first results of electronic transport experiments. At low temperature, the conductance is found to strongly depend on the strength and orientation of a magnetic field.

[1] Ch. Heyn et al., Appl. Phys. Lett. 98, 033105 (2011)

[2] Th. Bartsch et al., Phys. Rev. Lett. 108, 075901 (2012)

DS 12.16 Mon 17:00 Poster B1

Thermoelectric Transport Properties of GeTe Rich GeTe-Sb$_2$Te$_3$ Thin Films — •Felix R. L. Lange[1], Ernst-Roland Sittner[1], Karl Simon Siegert[1], Peter Jost[1], and Matthias Wuttig[1,2] — [1]I. Physikalisches Institut (IA), RWTH Aachen University, 52056 Aachen, Germany — [2]JARA - Fundamentals of Future Information Technology, RWTH Aachen University, Germany

Phase change materials (PCM) are a class of alloys that can be reversibly and rapidly switched between the amorphous and the crystalline state. Since these two states differ significantly in their physical properties such as reflectivity and resistivity they are well suited for future nonvolatile data storage applications. Some PCM along the pseudo-binary line between GeTe and Sb$_2$Te$_3$ exhibit a rather unusual combination of physical properties which render these alloys a potential *p*-type thermoelectric. These alloys allow access to a meta-stable cubic phase where one lattice site is randomly occupied by Ge, Sb and a certain amount of structural vacancies. Only recently Siegrist *et al.* identified disorder in these alloys as the cause of a metal to insulator transition. The degree of disorder can be affected by two independent parameters: stoichiometry and annealing conditions. Since disorder affects both, electrical and vibrational degrees of freedom, this opens up a pathway to tailor electrical and thermal transport properties independently. Using this concept we report enhanced thermoelectric efficiencies for GeTe rich GeTe-Sb$_2$Te$_3$ thin films prepared under different annealing conditions [1]. [1] E. R. Sittner *et al.*, *Phys Status Solidi* **A**, DOI 10.1002/pssa.201228397 (2012)

DS 12.17 Mon 17:00 Poster B1

Thermoelectric power factor and full ZT characterization of Bi2Te3-nanowires — •Rüdiger Mitdank[1], Danny Kojda[1], Zhi Wang[3], William Toellner[2], Kornelius Nielsch[2], Peter Woias[3], and Saskia F. Fischer[1] — [1]Novel Materials, Institute of Physics, Humboldt Universität zu Berlin, Newtonstr. 15, 12489 Berlin, Germany — [2]Institute of Applied Physics, Universität Hamburg, Jungiusstr. 11, 20355 Hamburg, Germany — [3]) IMTEK, University of Freiburg, D-79110 Freiburg

Thermoelectric (TE) properties of single Bi2Te3 nanowires (NW) were investigated using a TNCP (Thermoelectric characterization platform) which allows the determination of the Seebeck coefficient S, the conductivity σ and the thermal conductivity. The NW is deposited between 2 thin and freestanding Si-cantilevers. On each cantilever, 2 Pt-electrodes are arranged serving as microheater and thermometer. The calibration of the TNCP is discussed. In the temperature range 4,2K $<$ T $<$ 300K, the conductivity and the thermopower were measured. The function σ(T) corresponds to a rather metallic behaviour. The thermopower exhibits a maximum near 200 K. For a conductivity of nearly 1000S/cm the thermopower S(300K) varied between -35 μV/K and -50 μV/K. Experiments to determine the thermal conductivity are discussed.

DS 12.18 Mon 17:00 Poster B1

Thickness-dependent thermoelectric properties of BiSb thin films — •Heiko Reith[1,2], Friedemann Voelklein[2], and Michael Huth[1] — [1]Physikalisches Institut, Goethe-University, Frankfurt am Main, Germany — [2]IMtech, Hochschule Rhein Main, Ruesselsheim, Germany

We investigated the thermoelectric properties of BiSb thin films in the thickness range between 50 nm and 500 nm. For the determination of the thermoelectric properties we measured the Seebeck-coefficient and the thermal and electrical conductivity to obtain the figure of merit of the films. The thermal conductivity was measured using a specially designed microchip. For the electrical conductivity and Seebeck-measurement a four point structure deposited on a Si/Si$_3$N$_4$-wafer was used. The BiSb films were deposited onto these substrates using a thermal evaporation process. During the deposition of the films the substrates and microchips were placed next to each other and the thickness was detected by a quartz microbalance. Afterwards the thickness was measured with a surface profilometer. We present the used measurement techniques and results. From the measurement results we determine the figure of merit of the films and discuss the results using finite size effect models.

DS 12.19 Mon 17:00 Poster B1

Unexpected temperature dependence of thermal boundary conductance for epitaxial Bi(111) films on Si(001) — •Verena Tinnemann, Tim Frigge, Boris Krenzer, Anja Hanisch-Blicharski, Friedrich Klasing, Annika Kalus, and Michael Horn-von Hoegen — Faculty of Physics and Center for Nanointegration CENIDE, University of Duisburg-Essen, Lotharstr. 1, 47057 Duisburg, Germany

Ultrafast time-resolved reflection high energy electron diffraction was used to study the heat transfer from epitaxial Bi(111) films into the Si(001) substrate. Films with thicknesses in the range from 25 nm to 120 nm were prepared in-situ under UHV conditions. In a pump-probe setup the Bi films were excited by 50 fs-laser pulses with a wavelength of 800 nm. Short electron pulses were created by photoemission, accelerated to 7 keV, and focused by an electrostatic lens. For variable time delays between laser pump and electron probe diffraction patterns were recorded. The transient drop of spot intensity is explained in terms of the Debye-Waller effect and reflects the instant heating and subsequent cooling of the Bi films. The thermal boundary conductance of the interface is then determined from the exponential cooling of the film. We show that the thermal boundary conductance increases by more than 35% if the substrate temperature is increased from 80 K to 300 K. This is not explained by numerical simulations of the heat transport using temperature dependent parameters. For the 120 nm thick Bi-film a bi-exponential intensity is observed and explained by diffusion in the film and across the interface.

DS 12.20 Mon 17:00 Poster B1

Structural and electrical properties of thermoelectric $\mathrm{Fe}_x\mathrm{Co}_{1-x}\mathrm{Sb}_3$ thin films — Ayham Dalla, •Marcus Daniel, Andreas Liebig, Fabian Ganss, Gunter Beddies, and Manfred Albrecht — Chemnitz University of Technology, Institute of Physics

Increasing interest in efficiency enhancement of existing energy sources led to an extended research in the field of thermoelectricity. A suitable thermoelectric material like CoSb_3 is characterised by a high power factor and a low thermal conductivity. To control and improve the power factor a targeted electrical doping is necessary to achieve charge carrier densities up to 10^{20} cm^{-3}. In case of CoSb_3 controlled doping can be obtained by a partially substitution of Co by Fe atoms. In this study, 30 nm thick $\mathrm{Fe}_x\mathrm{Co}_{1-x}\mathrm{Sb}_y$ films have been deposited via MBE onto thermally oxidized Si(100) substrates at room temperature. The samples were post-annealed in ultra-high vacuum for one hour at 450°C. Two sample series with varying Fe content ($0<x<0.5$) were fabricated, a Sb rich ($y = 3.3$) and a Sb deficient series ($y = 2.5$). The composition was verified by RBS and the XRD analysis confirmed CoSb_3 as major phase. A systematic decrease of the extracted lattice parameter with increasing Fe content indicated the substitution of Co by Fe atoms. The electrical characterization was performed in a temperature range between 4 K and 300 K. Both series show an increase in charge carrier concentration with increasing Fe content, and thus a decrease in resistivity. The temperature dependence of the resistivity revealed for both sample series a change from semiconducting to metallic behaviour at a critical charge carrier concentration.

DS 12.21 Mon 17:00 Poster B1

Measurement setup fpr simultaneous determination of electrical conductivity, Hall coefficient and Seebeck coefficient. — •H. Kolb, J. de Boor, A. Sesselmann, T. Dasgupta, G. Karpinski, and E. Müller — DLR, Institute of Materials Research, Cologne

Thermoelectric materials can convert heat directly into usable electrical energy. An important aim in thermoelectric research is to find and optimize suitable materials and improve their performance to get higher efficiency. For a complete characterization it is in general required to do several different measurements in different apparatuses which can be challenging and time consuming. Therefore we developed a measurement system that can measure three of the thermoelectric key quantities (electrical conductivity, Seebeck- and Hall coefficient) simultaneously from room temperature up to 1000K, which is a typical temperature region for many potential applications of these materials. All three quantities are coupled via the charge carrier concentration and therefore a simultaneous measurement is important for a deep insight in the charge carrier transport in the sample. This is particularly important for thermally instable materials, where consecutive measurements can easily lead to misinterpretations. Four sheathed thermocouples arranged in a van der Pauw geometry are pressed by small springs on a round sample for electrical contact. This special arrangement allows for the electrical measurements, while the thermocouples allow for a determination of the Seebeck coefficient if an additional temperature gradient is applied. We will discuss technical details, features and limitations of the setup.

DS 12.22 Mon 17:00 Poster B1

Anomalous enhancement of the thermoelectric figure of merit by V co-doping in SrTiO_3 — •Udo Schwingenschlögl and Mousumi Upadhyay-Kahaly — KAUST, PSE Division, Thuwal, Saudi Arabia

The effect of V co-doping in Nb-SrTiO_3 and Pr-SrTiO_3 is studied by full-potential density functional theory. While in Nb-SrTiO_3 a high carrier density counteracts a high thermoelectric figure of merit, the trend is inverted by V co-doping. A similar but even more pronounced effect is found in Pr-SrTiO_3. The mechanism leading to this behavior is explained in terms of a local spin-polarization introduced by the V ions. Our results indicate that magnetic co-doping can be a prominent tool for improving the thermoelectric figure of merit.

Reference: Applied Physics Letters **100**, 193110 (2012)

DS 12.23 Mon 17:00 Poster B1

The effect of interfaces on the thermoelectric properties of laterally microstructured ZnO-based thin-films — •David Hartung, Florian Gather, Achim Kronenberger, Martin Eickhoff, Bruno K. Meyer, and Peter J. Klar — I. Physikalisches Institut, Justus-Liebig-University, Heinrich-Buff-Ring 16, 35392 Giessen

A series of samples was laterally microstructured with a self-aligned pattern transfer method consisting of alternating stripes of ZnO grown by molecular-beam epitaxy and radio-frequency sputtered Ga-doped ZnO stripes. The MBE-grown ZnO thin film samples were laterally microstructured by photolithography followed by ion-beam etching in order to obtain different lateral arrangements of stripes of defined interface geometry. In a second step the free regions between the stripes of MBE-grown ZnO were sputtered with Ga-doped ZnO. A lift-off step completes the micro-fabrication of a planar alternating ZnO/ZnO:Ga bar structure on each sample.

Throughout the series the bar width and hence the number of interfaces was kept constant, but the interface profile was varied yielding different interface lengths and geometries.

We measured in-plane as a function of temperature the Seebeck coefficient S and the electrical conductivity σ of the samples with the transport direction perpendicular to the stripe direction.

The measured data were compared to simulated data using an empirical network model.

DS 12.24 Mon 17:00 Poster B1

Thermoelectric properties of $\mathrm{ZnO}_{1-x}\mathrm{S}_x$ thin films — •Florian Gather, Achim Kronenberger, Peter J. Klar, and Bruno K. Meyer — I. Physikalisches Institut, Justus-Liebig-University, Heinrich-Buff-Ring 16, 35392 Giessen

We investigated the thermoelectric properties of rf-sputtered $\mathrm{ZnO}_{1-x}\mathrm{S}_x$ thin films on sapphire substrates. Due to its good availability and its non-toxicity, $\mathrm{ZnO}_{1-x}\mathrm{S}_x$ is a promising candidate for thermoelectric applications. The electric conductivity σ, the Seebeck coefficient S and carrier concentrations of a series of hydrogen doped samples and aluminum doped samples respectively were determined in in-plane direction over a wide temperature range. For the investigation of the influence of the sulphur concentration x on the thermal conductivity κ we employed the 3-omega method on a series of undoped thin-films. The measurements reveal a reduced κ in cross-plane direction of the samples containing sulphur compared to zinc-oxide samples. Using Raman spectroscopy we found indications for local phonon modes of oxygen in zinc-sulfide and of sulphur in zinc-oxide, respectively. These local phonon modes cause the reduction of κ observed in the experiments. Both sample series are compared in terms of crystal quality and grain size using XRD-analysis and atomic force microscopy.

DS 13: Poster Session III: Layer properties: electrical, optical and mechanical properties; Thin film characterization: structure analysis and composition (XRD, TEM; XPS, SIMS, RBS..)

Time: Monday 17:00–20:00 Location: Poster B1

DS 13.1 Mon 17:00 Poster B1

Characterisation of YSZ thin films deposited by RF sputtering — •Daniel Reppin[1], Markus Piechotka[1], Jens Peter Eufinger[2], Benjamin Pachner[1], Angelika Polity[1], Peter J. Klar[1], Bruno K. Meyer[1], and Jürgen Janek[2] — [1]1. Physikalisches Institut, Justus-Liebig-Universität, Heinrich-Buff-Ring 16, 35392 Giessen — [2]Physikalisch-Chemisches Institut, Justus-Liebig-Universität, Heinrich-Buff-Ring 58, 35392 Giessen

Yttria-stabilised zirconia (YSZ) is a technically widely used oxygen ion conductor employed for example in oxygen sensors and solid oxide fuel cells. For these applications the film properties such as the crystal structure and ion conductivity are of major interest. YSZ thin films were deposited from a ceramic target with 9.5 mol% Y_2O_3 by RF sputtering on silicon (004) and fused silica substrats. The films were investigated by 4-circle XRD measurements to determine whether the crystal structure is cubic or tetragonal. Scanning electron microscopy was used to inspect the grain size of the films. Impedance spectroscopy measurements were performed to quantify the oxygen ion conduction.

DS 13.2 Mon 17:00 Poster B1

Doped TiO_2 as alternative transparent conducting oxide — •Daniel Dorow-Gerspach, Philipp Schulte, Patrick Ries, and Matthias Wuttig — I. Physikalisches Institut (IA) RWTH-Aachen University

In many highly demanded modern devices, such as displays and solar cells, materials are needed, that are transparent and at the same time highly conductive. Commonly such materials are called transparent conducing oxides (TCO), with the well-known and efficient but also expensive representative In_2O_3:Sn. A promising cheaper alternative is Niobium doped Titania (TiO_2:Nb), with the matrix material TiO_2 that is already used for anti-reflective coatings or self-cleaning surfaces. For the commercial utilization, there are two challenges. One is the relatively high temperature for the annealing of amorphously deposited TiO_2. The other challenge is that the most conducting films were achieved by RF-sputtering, which is not suitable for large scale production processes. In this work we have used TiO_2 seed layers to reduce the required annealing temperature by 50 K. To address the second point and obtain higher deposition rates, we have employed a reactive DC-sputtering process using a metallic Ti:Nb target. These approaches led to the fabrication of conducting films with a reduced crystallization temperature yet good electronic properties.

DS 13.3 Mon 17:00 Poster B1

Prozess characteristics and film properties upon doping of TiO_2 by reactive serial co-sputtering utilizing high power impuls magnetron sputtering — •Rüdiger M. Schmidt[1], Oliver Lenck[2], Tomas Kubart[3], Dominik Wagner[1], Andreas Pflug[2], Thomas Nyberg[3], Sören Berg[3], and Matthias Wuttig[1] — [1]I. Institute of Physics, RWTH Aachen University, Germany — [2]Fraunhofer IST, Braunschweig, Germany — [3]Solid State Electronics, The Ångström Laboratory, Uppsala University, Sweden

Titanium Dioxide (TiO_2) is a material with attractive properties which have led to various applications such as anti-reflective coatings or self cleaning surfaces. High power impulse magneton sputtering (HiPIMS) is a PVD technique in which the power is applied to the target with low duty cycle (<10%) and frequenzy (<10 kHz) resulting in a high degree of ionization of the sputtered species. As a result, films deposited by HiPIMS show smooth surfaces and high densities. Unfortunatly the deposition of TiO_2 using HiPIMS is hampered by significantly lower deposition rates compared to dcMS. Sputter Yield Amplification (SYA) can be used, through recoil of the sputtering species at implanted heavy dopants below the target surface, to increase deposition rates. We have built a designated sputter deposition tool which enables systematic studies of different dopants. In this study TiO_2 is doped with Tungsten and Tantalum resulting in a rate increase of 250-400% and 180-320% respectively. Optical measurements in the visible range show that the absorption of TiO_2:Ta is less than 0.5%, whereas TiO2:W shows a somewhat higher absorption.

DS 13.4 Mon 17:00 Poster B1

Influence of doping on the metal-semiconductor transition of VO_2 thin films — •Marc K. Dietrich, Angelika Polity, Benedikt Kramm, and Bruno K. Meyer — Justus-Liebig-Universität Gießen, I. Physikalisches Institut, Heinrich-Buff-Ring 16, 35392 Gießen, Germany

The optical and structural properties close to the metal-semiconductor transition of doped vanadium dioxide (VO_2) films have been investigated. Doped VO_2 thin films were deposited by rf sputtering technique on TiO_2 coated glass substrates. Single crystal VO_2 undergoes a phase transition near 68°C, while doping (e.g. fluorine and tungsten) decreases the transition temperature. Therefore, VO_2 has potential for many applications involving thermally activated optical or electronic switching devices. For an application as window coating which switches the transmission dependent on the ambient temperature the determination of luminous transmittance and the g-value are of substantial importance. We determined these properties for the switching in the range of the ambient temperatures.

DS 13.5 Mon 17:00 Poster B1

Optical and magnetotransport properties of ZnO thin films grown by metalorganic aerosol deposition — •Christoph Meyer, Sebastian Hühn, Markus Jungbauer, Markus Michelmann, and Vasily Moshnyaga — I. Physikalisches Institut, Georg-August-Universität Göttingen

ZnO, a II-IV semiconductor with a wide direct bandgap $E_g = 3,4$ eV and a near UV and blue photoluminescence zone, is a promising material for optoelectronic, spintronic and photovoltaic applications, which due to recent successes in nanoscale science, becomes even more attractive today. Therefore a growth control of ZnO thin layers on commercially available substrates as well as a control of doping with n- and p-type dopants or magnetic transition metals is an absolutely necessary task. In this work the photoluminescence and Raman spectroscopies are used to detect and identify typical impurity- and dopant-related optical transitions in ZnO layers, grown by metalorganic aerosol deposition (MAD). The growth conditions (e.g. temperature, deposition rate or precursor molarity) and the substrates (Al_2O_3, MgO buffered Al_2O_3, ZnO) were varied to improve the quality of the layers. Standard sample characterization techniques, e.g. AFM, XRD, SQUID and Hall effect, were used additionally to confirm the quality of the films. XRD reveals c-axis oriented ZnO films on Al_2O_3(0001) substrates. We observed a room temperature photoluminescence caused by exciton transition at $E = 3,288$ eV as well as phonon replica.

DS 13.6 Mon 17:00 Poster B1

Synthesis, microstructure and local electronic conductivity of platinum/titanium oxide contacts — •Marian Bongers, Astrid Pundt und Carsten Nowak — Institut fuer Materialphysik, Friedrich-Hund-Platz 1, 37077 Goettingen, Germany

Pt/TiO_x Schottky contacts are of interest for surface chemical reactions as they allow measuring hot electrons, show catalytic activity and exhibit a change in there electronic characteristics under different chemical ambient. As these effects depend on the crystallographic orientation, a careful characterization of the microstructure is required.
Here we present studies on the growth of TiO_2/Pt double layers on MgO <100> single crystals. Layers with several hundred nanometers thickness were prepared by reactive atom beam sputter deposition under O_2 and Xe atmosphere. The layers were structurally characterized by XRD, EBSD and AFM. For optimized synthesis temperature the investigations revealed a preferred <100> orientation of the Pt layer with lateral grain size of the order of 100 μm. For the TiO_2 layers a polycrystalline microstructure was observed. Local I-V-characteristics were measured with conductive AFM and tungsten tips of μm size, revealing rectifying behavior.
Further, investigations on the influence of the deposition temperature and thermal annealing on the quality of the TiO_2 layers are presented. The influence of a chemical gas ambient on the I-V-characteristics of the synthesized Pt/TiO_x contacts will be discussed.
Fincanial support by the DFG via projects PU131/9 and SFB602 is gratefully acknowledged.

DS 13.7 Mon 17:00 Poster B1

Enhanced wear resistance of a rhodium surface by interstitial alloying with boron — •Frank Müller[1], Matthias Lessel[1], Samuel Grandthyll[1], Karin Jacobs[1], Stefan Hüfner[1], Stefan Gsell[2], Michael Weinl[2], and Matthias Schreck[2] — [1]Saarland University, Experimental Physics, 66041 Saarbrücken, Germany — [2]University of Augsburg, Institute of Physics, 86135 Augsburg, Germany

Increasing the wear resistance of a Rh(111) surface can be obtained by ~ 1% alloying with boron atoms via a CVD (Chemical Vapour Deposition) process using trimethylborate, B(OCH3)3, at moderate temperatures of about 800 K. The fragmentation of the precursor molecules on the metal surface results in single boron atoms that are incorporated in the fcc lattice of the substrate, as displayed by X-ray Photoelectron Diffraction (XPD). The boron atoms penetrate into the host lattice up to 100 nm with the boron distribution displaying a nearly homogeneous depth profile, as tested by depth profiling experiments using combined X-ray photoelectron spectroscopy (XPS) and Ar ion etching. When compared to the untreated Rh(111) surface, the wear resistance of the B-"doped" Rh surface is increased to about 400%, as probed by scratching experiments using Atomic Force Microscopy (AFM).

DS 13.8 Mon 17:00 Poster B1

Stress induced wrinkling in laser deposited polymer/metal-nanocomposites — •Anja Westphal, Susanne Schlenkrich, Felix Schlenkrich, Stephanie Demuth, and Hans-Ulrich Krebs — Universität Göttingen, Institut für Materialphysik, Friedrich-Hund-Platz 1, D-37077 Göttingen

Wrinkling of metal surfaces with different periodicities on the nanometer scale can be obtained by pulsed laser deposition (PLD, 248 nm, pulse duration of 30 ns) of polymer/metal bilayers directly after preparation. Systematically, the thickness dependence of the morphology and topography of the wrinkled metal films was analyzed by electron microscopy (SEM) and atomic force microscope (AFM). The characteristic wave lengths were determined by fourier transformation of the AFM surface patterns. Using the beam theory these wavelengths can be related to the tensile moduli of both film components, and the thicknesses of the polymer and metal film, respectively. The early growth stages were also studied by resistance measurements in order to find the transition from isolated metal clusters to closed layers while increasing the amount of metal. The origin of the stress induced wrinkling induced in the metal layers during PLD, the changes in wavelength and a possible application for the measurement of the elastic moduli of thin films will be discussed.

DS 13.9 Mon 17:00 Poster B1

Preparation of equiatomic FeRh thin film by MBE — •Alireza Heidarian[1,2], Kay Potzger[1], Jürgen Lindner[1], and Rantej Bali[1] — [1]HZDR Institute of Ion-Beam Physics and Materials Research P.O. Box 510119, 01314 Dresden, Germany — [2]TU Dresden Helmholtzstr. 10, 01069 Dresden, Germany

High quality equiatomic FeRh thin films with varying thickness have been prepared on MgO (100) substrates via molecular beam epitaxy (MBE). The optimization of the stoichiometry was monitored using XRD, RBS and AES while the magnetic properties were probed in a SQUID. XRD results evidence a well-ordered CsCl-type crystal structure. By increasing the annealing temperature of the films, the structural quality of the films also increase. Moreover, the known first order phase transition at ~350 K from an antiferromagnetic (AF) to a ferromagnetic (FM) state slightly shifts towards higher temperatures. M-H loops of films annealed at 800 °C or 850 °C recorded at 300 K show an opening, which is likely related to the magnetic field-induced AFM-FM phase transition[1]. Residual low-temperature ferromagnetic moments are related to disorder or Fe diffusion towards the interfaces.[1] J. Cao, T. Nam, N. Phuoc and T. Suzuki. J. Appl. Phys 103, 07F501 (2008).

DS 13.10 Mon 17:00 Poster B1

Semiconducting thin films processed at low temperatures from unstabilized ZnO nanoparticle solutions — •Paul Mundt[1], Nicole Anderl[2], and Heinz von Seggern[1] — [1]Electronic Materials Division, Institute of Materials Science, Technische Universität Darmstadt, Petersenstr. 23, 64287 Darmstadt, Germany — [2]Ernst-Berl-Institut für Technische und Makromolekulare Chemie, Technische Universität Darmstadt, Petersenstrasse 22, D-64287 Darmstadt, Germany

Recently, zinc oxide nanoparticles (ZnO-NP) have become a subject of considerable interest due to their properties showing a high potential for developing solution processed, low cost, low temperature semiconducting devices. Most of the work so far uses sterically stabilized ZnO-NP dispersions. However, the stabilizing agents can have a negative impact on the electronic properties of the resulting semiconducting thin film. They act as additional barriers for the charge carriers. Removing these stabilizers from the film usually requires high temperature treatments being not compatible with flexible polymeric substrates. The present work utilizes sol gel processed ZnO-NPs without an additional steric stablization. Thin ZnO-NP films are produced by spin coating and characterized by various techniques to obtain information about the crystallographic structure, the band energies and the topography. Additionally, thin film transistors with a ZnO-NP active layer processed at temperatures of 150°C only and therefore suitable for applications on flexible substrates are realized yielding electron mobilities of 10^{-3}cm^2/Vs.

DS 13.11 Mon 17:00 Poster B1

Epitaxial Fe_3O_4/NiO bilayers grown on MgO(001) — •Tobias Schemme[1], Florian Bertram[2], Karsten Kuepper[1], and Joachim Wollschlaeger[1] — [1]Fachbereich Physik, Universitaet Osnabrueck, Barbarastr. 7, 49076 Osnabrueck — [2]HASYLAB, DESY, Notkestr. 85, 22607 Hamburg

The investigation of magnetic interactions at the interface of thin films is of huge physical and technological interest for instance for the development of magnetoresitive (MR) devices. Epitaxial Fe_3O_4/NiO bilayers were grown on MgO(001) substrates. First, a film of NiO was deposited on the substrate using molecular beam epitaxy (MBE) at 250°C in a 10^{-5} mbar oxygen atmosphere. Afterwards a magnetite film was deposited on the NiO film via reactive MBE at the same temperature. In this study, bilayers with different NiO thicknesses but constant magnetite thickness were investigated. The stoichiometric composition of the oxide films was investigated by X-ray Photoelectron Spectroscopy (XPS), while the thickness and structure were examined by X-ray Diffraction (XRD) and Low Energy Electron Diffraction (LEED), respectively. Structural characterizations indicate a perfect epitaxy of the films. The LEED patterns of the magnetite films show the typical $(\sqrt{2}\times\sqrt{2})$R45° superstructure, while the LEED patterns of the NiO films show the expected (1×1) structure. X-ray Reflectometry (XRR) and XRD measurements were used to quantify the increasing thickness of the NiO films and to validate the crystallinity of the bilayer. The stoichiometric analysis via XPS proofs that the bilayer films consist of stoichiometric Fe_3O_4 and NiO.

DS 13.12 Mon 17:00 Poster B1

Thick manganite films grown by MAD — •F. Fischgrabe[1], E.S. Zhukova[2,3], B. Gorshunov[2,3], M. Dressel[3], and V. Moshnyaga[1] — [1]I. Physikalisches Institut, Universität Göttingen, Germany — [2]Prokhorov General Physics Institute, Russian Academy of Sciences,Moscow, Russia — [3]I. Physikalisches Institut, Universität Stuttgart, German

We report preparation and characterization of $La_{1-x}Ca_xMnO_3$ (LCMO) x=0,3-0,5 films with thickness $1-10\mu m$. Thick epitaxial manganite films could be interesting for THz as well as for far IR Fourier spectroscopy measurements, aimed to study low-energy excitations, like CDW and folding phonons, important for the manganite physics. The samples were grown using metalorganic aerosol deposition (MAD) technique. To verify the film quality XRD, DC and AC resistivity (f=0,1Hz-40MHz; T=5-300K), STM, REM and THz measurements were carried out. $1\mu m$-thick LCMO films with x=1/3 show a metal-insulator transition at T=272 K and residual resistivity, $\rho(5K) \approx 10^{-4}\Omega cm$, i.e. the values characteristic for thin epitaxial LCMO films. XRD measurements demonstrate out-of-plane texture with c=0.3864 nm very close to the bulk value as well as single phase composition. The results show the MAD potential to produce high quality thick oxide films for industrial applications, like coating conductors.

DS 13.13 Mon 17:00 Poster B1

Temperature and time dependent *in-situ* crystallization of strontium titanate thin films — •Florian Hanzig[1], Carsten Richter[1,2], Juliane Hanzig[1], Erik Mehner[1], Hartmut Stöcker[1], Barbara Abendroth[1], and Dirk C. Meyer[1] — [1]TU Bergakademie Freiberg, Institut für Experimentelle Physik — [2]HASYLAB bei DESY, Hamburg

Strontium titanate is a well-known transition metal oxide crystallizing in the perovskite type of structure. With its large band-gap and its mixed ionic and electronic conductivity, $SrTiO_3$ is a promising isolating material in metal-insulator-metal (MIM) structures for resistive switching memories. In this paper, the crystallization of amorphous strontium titanate thin films is investigated by *in-situ* grazing incidence x-ray diffraction using synchrotron light (Beamline E2 at DORIS III - HASYLAB / DESY, Hamburg). We focus on the crystallization mechanisms in dependence of the layer stoichiometry and heating rates. Different physical vapour deposition methods have been used to fabricate stoichiometric and Sr-rich layers. The crystallization and evolution of phase composition, crystallite size and strain of the $SrTiO_3$ layers were investigated for temperatures up to 950 °C under atmospheric conditions. At approximately 350 °C crystallization of the perovskite-type $SrTiO_3$ is initiated for Sr-rich electron beam evaporated layers, whereas stoichiometric sputter deposited thin films crystallize from about 500 °C. During annealing a diffusion of Si from the substrate into the $SrTiO_3$ layer occur leading to the formation of secondary silicate phases which are detected by XPS.

DS 13.14 Mon 17:00 Poster B1

Bayesian Fitting of Neutron and X-Ray Reflectivity Data — •Jean-Francois Moulin, Martin Haese-Seiller, and Andreas Schreyer — Helmholtz-Zentrum Geesthacht Boltzmann Strasse 1 21502 Geesthacht Germany

Deducing the structure of thin films by analysis of the X-ray or neutron reflectivity curves often proves to be challenging. The inversion problem does not have a unique solution and the $\chi 2$ landscape which has to be searched for a global minimum is often very unfavorable to the use of standard techniques such as the Levenberg-Marquardt algorithm. It is well known that human guidance is often required in order to start the search with a parameter set which is already very close to the real solution. In the quest for better fitting methodologies many efforts have been devoted to techniques which garantee that the algorithm does not get stuck in local minima. Notable examples are genetic algorithms, particle swarm optimisation and Bayesian analysis. Bayesian optimization makes use of a Monte Carlo exploration of the $\chi 2$ landscape and eventually leads to a description of the parameters corelations and the distributions of their values. In the Bayesian framework one encodes all a priori knowledge about the experiment and then extracts from the posterior data a quantitative information about what we can learn from the experimental observation. In this paper we will show how one can take advantage of the Bayesian optimization methods to charachterize thin films and we will demonstrate the use of readily available open source libraries to build an efficient and reconfigurable toolbox which can tackle a variety of problems.

DS 13.15 Mon 17:00 Poster B1

Laser-induced phase transitions in PLD-deposited Ge2Sb2Te5-films using single nanosecond UV-pulses — •Erik Thelander[1], Hongbing Lu[1,2], Ulrich Ross[1], Jürgen Gerlach[1], and Bernd Rauschenabch[1] — [1]Institute of Surface Modification, Leipzig, Germany — [2]Hubei University, Wuhan, China

Phase transformations between amorphous and metastable crystalline state were induced by irradiation with a 248 nm single nanosecond pulse in films grown with pulsed laser deposition. By adjusting the laser fluence, the two different phases were obtained and could be distinguished by differences in optical reflectivity. Detailed structural analysis was carried out with XRD and HRTEM to elucidate the effect of laser fluence on the crystalline nature of the samples. Large structural differences between laser-annealed and thermally annealed films were revealed, in terms of lattice constant expansion and grain size evolution. This is believed to originate from the fast heating rate and short duration of the laser pulse. X-ray reflectivity measurements showed a 3.58 % densification upon laser-induced crystallization.

DS 13.16 Mon 17:00 Poster B1

Microstructural investigation of epitaxial grown GaN thin films using hyperthermal ions — •David Poppitz, Andriy Lotnyk, Jürgen W. Gerlach, and Bernd Rauschenbach — Leibniz-Institut für Oberflächenmodifizierung e. V., Permoserstr. 15, D-04318 Leipzig

Gallium nitride thin films grown with ion beam assisted molecular beam epitaxy on different substrates and at different growth parameters are studied by using (S)TEM imaging and chemical analysis. The aim of this study is to get information about the interface between gallium nitride film and the substrate materials using high resolution TEM. The gallium nitride thin films were grown on 6H-SiC(0001) and Al2O3(0001) substrates without using buffer layers. The influence of the substrate temperature in the range from 630 °C to 750 °C and the nitrogen ion/gallium flux ratio on the growth process is investigated. The aim was to examine the defect structure of the films with a high resolution Cs-corrected analytical TEM. To get high resolution pictures sensitive and sophisticated preparation methods were used and optimized relating to the material system. TEM lamellae were sliced by using focused ion beam technique and afterwards the samples were thinned by ultra-low energy argon ion polishing. In this process amorphous layers and gallium implementations from the cutting process with high energetic gallium ions were removed. Very thin sample thicknesses of a few nanometers have been achieved and high resolution (S)TEM images could be taken. Further chemical analysis at the nanometer scale by using EDX- and EELS- measurements were done.

DS 13.17 Mon 17:00 Poster B1

Quantitative investigation of laser-deposited Ge2Sb2Te5 by abberation corrected STEM/EELS — •Ulrich Ross, Andriy Lotnyk, Erik Thelander, and Bernd Rauschenbach — Leibniz-Institut für Oberflächenmodifizierung e.V. Permoserstr. 15 D-04318 Leipzig

We have investigated amorphous as well as crystalline Ge2Sb2Te5 thin films grown by pulsed laser deposition onto various substrates, utilizing the capabilities of an analytical TEM (Titan 80-300kV Cs probe corrected) in conjuncture with a post-column EELS spectrometer. The material system Ge2S2bTe5 (GST) is of special interest as a test-case for phase-change behaviour materials. As such, we have investigated both as-deposited as well as recrystallized thin-film samples in regards to local composition, local crystallinity and crystal structure. In addition, we aim to make use of the excellent spacial and energy resolution of the Cs-corrected STEM-EELS in order to correlate local composition with changes in the conduction behaviour characteristic for phase-change materials. Preliminary results will be presented, illustrating quantitative high-resolution STEM as a promising approach to futher understanding of the physical phenomena behind phase-change behaviour.

DS 13.18 Mon 17:00 Poster B1

Epitaxy of Ultrathin Metal Films for Ultrafast Electron Diffraction and Plasmonics — •T. Becker, S. Meyer, T. Payer, F.-J. Meyer zu Heringdorf, and M. Horn-von Hoegen — University Duisburg-Essen, Duisburg, Germany

Monocrystalline metal films on halogenide salt substrates and mica were epitaxially grown to produce electron transparent, free-standing membranes with few 10 nm thickness for ultrafast transmission electron diffraction respectively thicker films for use in plasmonic excitation. Au, Co and Fe films with various thicknesses from 20 nm to 100 nm were deposited under UHV conditions by molecular beam epitaxy in a temperature range from -100 °C to 470 °C on clean and atomically plain NaCl or KCl substrates that were prepared as described in [1]. The mica substrates were cleaved. The morphology was examined using in-situ LEED and ex-situ AFM. Cobalt forms 3D islands in the μm-regime. Continuous iron films with a rms surface roughness of less than 1 nm were obtained after annealing at 330 °C for one hour. For Au on KCl another type of growth was observed. In the whole temperature range 3D islands with different diameters and heights up to 140 nm are dominating the surface structure. To obtain closed monocrystalline Au films with rms surface roughness below 1 nm, Au was deposited at 250 °C on a mica substrate.

[1] T.Payer et al., Appl. Phys. Lett. 93, 093102 (2008)

DS 13.19 Mon 17:00 Poster B1

Formation of ZnO layers by spraying Zn(acac)2 and [Zn(O2C(CH2OCH2)3H)2] precursors from solution — •Iulia G. Toader[1], Falko Seidel[1], Philipp Schäfer[1], Ovidiu D. Gordan[1], Alexander Jakob[2], Stefan Möckel[2], Heinrich Lang[2], Michael Hietschold[3], 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-09111 Chemnitz, Germany — [3]Solid Surfaces Analysis Group, Chemnitz University of Technology, D-09107 Chemnitz, Germany

Due to its transparency and wide band gap ZnO represents a suitable material for future transparent electronics. In this work, two ZnO precursors namely zinc acetylacetonate hydrate (Zn(acac)2) and zinc(II)-[2-(2-methoxyethoxy)ethoxy]acetate ([Zn(O2C(CH2OCH2)3H)2]) were sprayed from solution. A post annealing treatment was applied on the as-sprayed films which led to the formation of ZnO layers. Their investigation was performed using infrared and Raman spectroscopies, scanning electron microscopy, and energy dispersive X-ray spectroscopy. By varying parameters such as the heating temperature and the time interval during heating, the quality of the ZnO layers formed could be tested and improved. It was therefore proven that not only the temperature but most importantly the heating time play an important role in achieving high quality ZnO layers. Moreover, it was shown that for the two precursors the same heating treatment leads to completely different film morphologies.

DS 13.20 Mon 17:00 Poster B1

Photoemission Analysis of PLD grown Oxide Heterointerfaces — •Uwe Treske, Andreas Koitzsch, Martin Knupfer, and Bernd Büchner — Institute for Solid State Research, IFW-Dresden, P.O.Box 270116, D-01171 Dresden, Germany

Pulsed laser deposition enables monolayer controlled growth of transition metal oxide heterointerfaces with a variety of exotic phenomena depending on the growth conditions. A prominent example is the formation of a high-mobility two-dimensional electron gas at the interface of LaAlO$_3$ grown on TiO$_2$-terminated SrTiO$_3$ substrates. The origin of conductivity at the interface of such insulating oxides is still under discussion. The polar catastrophe, oxygen vacancies and also cation intermixing should be taken into account. We apply soft x-ray photoemission studies to investigate stoichiometric aspects as well as in-gap states and differences in the core levels depending on the layer thickness.

DS 13.21 Mon 17:00 Poster B1

Direct observation of deuterium-dead layer in Fe/V multilayers by atom probe tomography — •Ryota Gemma[1,2], Talaat Al-Kassab[2], Reiner Kirchheim[1], and Astrid Pundt[1] — [1]Institute of Materials Physics, University of Göttingen, Friedrich-Hund-Platz 1, D-37077 Göttingen, Germany — [2]Physical Science and Engineering Division, King Abdullah University of Science and Technology (KAUST), Thuwal 23955-6900, Kingdom of Saudi Arabia

Atom probe tomography (APT) is nowadays regarded as one of the promising tools to analyze hydrogen or deuterium (D) distributions on the atomic scale. At metallic hetero-interfaces, it has been suggested that a nanometer thin hydrogen-dead layer (DL) appears due to an interface charge transfer and/or to an elastic discontinuity. With focus on such an interface effect, we investigated the local deuterium distribution in multilayered thin Fe/V films by APT. More recently, we have succeeded to observe DL by APT. In this contribution, we report on detailed studies on DL: The DL in Fe/V multilayers can be successfully separated from an interface mixing effect. The observed DL thickness commonly ranges from 0.4 to 0.5 nm, showing an excellent agreement with the previously suggested DL thickness. But, the DL is found to disappear at high deuterium concentrations above 0.1 D/Metal. This is considered to originate from occupation of high energy interstitial sites by D atoms, at the interface. A sloped plateau region as found in the corresponding p-c-T diagram, supports this interpretation. Financial support by the DFG via project PU131/9 is gratefully acknowledged.

DS 13.22 Mon 17:00 Poster B1

Construction of a multichromatic dual-beam magnetometer using a triaxial magnetic field based on the magnetooptic Kerr effect — •Gerhard Götz, Timo Kuschel, and Günter Reiss — University of Bielefeld, Germany

In this work we present the construction and optimization of a home-built magnetometer for investigations of the magnetic properties of thin films via the magnetooptic Kerr-Effect (MOKE). Based on a dual-beam system the polar MOKE as well as the quadratic MOKE can be measured seperately without contribution of the longitudinal MOKE using perpendicular incidence. The magnetic field can be applied in three dimensions to magnetize samples with in-plane or out-of-plane magnetization. The sample can be rotated around the sample normal to examine its in-plane anisotropy. Also the magnetization reversal process of in-plane and out-of-plane magnetized samples can be reconstructed and characterized by vectorial magnetometry via MOKE measurements using s- and p-polarized incident light and different magnetic field directions. Four laser diodes are used to study the linear and the quadratic MOKE spectrally using different wavelengths for the incident light in the visible range.

All this measurement modi are demonstrated in this work using Permalloy, Fe_3O_4 and $(CoFe)_{77}Tb_{23}$ thin films.

DS 14: Focus Session: Functionalized Semiconductor Nanowires I (jointly with HL)

Nanowires are filamentary crystals with a diameter ranging from few to hundred nanometers. Thanks to their special morphology and geometry, they are at the base of many applications that can revolutionize this century's technology. For this to become a reality, fundamental studies on the growth and properties are essential. This focus session presents the latest developments and discoveries in the area of nanowires, with a special focus on semiconductor materials. (Organizers: Margit Zacharias, U. Freiburg; Tobias Voss, U. Bremen; Anna Fontcuberta i Morral, EPFL)

Time: Tuesday 9:30–12:45 Location: H8

Invited Talk DS 14.1 Tue 9:30 H8

Nanowire photovoltaics with absorption beyond the ray optics limit. — •Magnus T Borgström — Solid state physics, Lund University, Lund, Sweden

Semiconducting nanowires have been recognized as promising materials for high-performance electronics and optics where optical and electrical properties can be tuned individually. The feasibility of III-V nanowire integration with existing silicon processing technology due to the small footprint between the silicon substrate and the nanowire material has further sparked that interest. For NWs to provide the new architecture for next generation photovoltaics there is a strong need to take complete control over synthesis. By optimizing growth conditions with respect to tapering we created nanowire-InP nanowire based solar cells using Au seed particles for growth. The nanowires were processed as-grown with a transparent top contact to create 1x1 square mm devices, with about 4 million nanowires contacted on each device. The solar cells were investigated under 1 sun (AM 1.5) illumination, and the devices show efficiencies higher than 10% and conversion of the solar irradiation into photocurrent beyond the ray optics limit.

Invited Talk DS 14.2 Tue 10:00 H8

Crystal structure control in nanowires — •Erik Bakkers — Eindhoven University of Technology, Den Dolech 2, 5612 AZ Eindhoven, The Netherlands — Delft University of Technology, Lorentzweg 1, 2600 CL Delft, The Netherlands

Important semiconductors like Si, Ge and GaP have an indirect bandgap when having the (normal) cubic crystal structure. It has been predicted that when these materials crystallize in a hexagonal structure that they can have a direct bandgap. But, these materials have never been controllably made with the pure wurtzite structure. Nanowires can be grown in other crystal structures than known in the bulk, offering new routes to tailor the optical and electronic properties. The nanowire growth mechanism will be discussed and the fabrication of the pure hexagonal form will be investigated. Here, we exploit these possibilities and discuss control of the crystal structure of nanowires and investigate the optical properties. Finally, we demonstrate the direct nature of the bandgap of wurtzite materials.

Topical Talk DS 14.3 Tue 10:30 H8

Spectral and spatial overlap of oxide quantum wells and whispering gallery modes — •Marius Grundmann — Universität Leipzig, Insitut für Experimentelle Physik II

We present the fabrication of zinc oxide nano- and microwires and the epitaxial growth of oxide heterostructures and quantum wells around the zinc oxide cores in radial direction. (Mg,Zn)O/ZnO and (Cd,Zn)O/ZnO QWs are compared and found to not exhibit quantum confined Stark effect, as expected for the non-polar growth directions. Due to the hexagonal cross-section, the ZnO wires exhibit whispering gallery resonances. The spectral and spatial overlap of the quantum wells with the whispering gallery modes is achieved in various geometries. The coupling of exciton and photon modes will be discussed.
This work was conducted together with C.P. Dietrich, M. Lange, T. Böntgen and M. Stölzel and financially supported by DFG in the framework of FOR1616 and by ESF.

Coffee break (15 min)

Topical Talk DS 14.4 Tue 11:15 H8

Semiconducting Nanowire Heterostructures on Silicon - From Growth to Devices — Heinz Schmid, Kirsten Moselund, Cedric Bessire, Pratyush Das Kanungo, Philipp Mensch, Siegfried Karg, Mattias Borg, Volker Schmidt, and •Heike Riel — IBM Research - Zurich, Rüschlikon, Schweiz

Bottom-up grown nanowires (NWs) are very attractive materials for direct integration of III-V semiconductors on Si thus opening up new possibilities for the fabrication and design of electronic and optoelectronic devices. The NW geometry allows the growth of abrupt heterostructures with large lattice mismatch and offers an ideal geometry for field-effect transistors (FETs) from an electrostatics perspective. These characteristics are especially important for tunnel FETs (TFETs) which today are being considered the most promising steep-slope devices. TFETs can achieve a subthreshold swing of less than 60 mV/dec and are thus attractive for low-voltage operation thereby offering significant power dissipation savings. We present our results on the fabrication and characterization of vertical InAs-Si heterojunction nanowire (NW) Esaki tunnel diodes and TFETs with InAs as low bandgap source. InAs NWs are grown on Si <111> by selective area epitaxy within e-beam patterned SiOx openings by MOCVD where the doping level is controlled in-situ. Furthermore, a new approach based on nanotube templates has been developed to grow axial III/V nanowire homo- and hetero-structures on silicon with high quality. The device fabrication will be discussed and the latest electrical results of tunnel diodes and TFETs will be presented.

Topical Talk DS 14.5 Tue 11:45 H8

III-nitride nanowires: From growth phenomena to light-emitting diodes — •Raffaella Calarco — Paul-Drude-Institut für Festkörperelektronik, Hausvogteiplatz 5-7, 10117 Berlin, Germany

Epitaxy in the form of freestanding vertical nanowires offers compared to planar layers the advantage that the interface between adsorbate and substrate is very small and that strain caused by lattice mismatch can elastically relax at the free sidewalls. Hence, dissimilar materials can be combined in high structural quality, and arguably the most relevant case is the growth of III-V compound semiconductors on Si substrates. We grow GaN nanowires on Si substrates by molecular beam epitaxy (MBE) and investigate nanowire properties that are essential for optoelectronic applications. Light emitting diodes (LEDs) have been fabricated using ensembles of free-standing (In, Ga)N/GaN NWs grown on Si substrates in the self-induced growth. Several characterization techniques indicate that the electroluminescence of such LEDs is governed by the differences in the individual current densities of the single-NW LEDs operated in parallel, i.e. by the inhomogeneity of the current path in the ensemble LED. In addition, the optoelectronic characterization leads to the conclusion that these NWs exhibit N-polarity and that the (In, Ga)N quantum well states in the NWs are subject to a non-vanishing quantum confined Stark effect. LEDs require NW ensembles with very homogeneous properties. Here, we present our selective area growth strategy for the synthesis of high-quality GaN NWs on prepatterned Si(111) substrates.

Topical Talk DS 14.6 Tue 12:15 H8

3D GaN nanorods: fabrication, properties, applications — •Andreas Waag, Johannes Ledig, Xue Wang, Milena Erenburg, Jana Hartmann, Lorenzo Caccamo, Matin Mohajerani, Manal Ali Deeb, Jiandong Wei, Martin Hoffmann, Hao Shen, and Hergo-Heinrich Wehmann — TU Braunschweig

GaN nanorods and 3D columns recently attracted a lot of attention since they are expected to be an exciting new route towards light engines for solid state lighting. In contrast to a planar thin film technology, a completely 3-dimensional nano- or microrod approach gives more freedom in the device design. E.g., a core-shell design of LEDs based on 3D GaN offer a dramatically enhanced active area per wafer footprint, since the active area is scaling with height of the 3D structures. High quality core-shell devices will have a tremendous impact on LED technology. However, there are also challenges related to a 3D device approach. Conventional planar characterization as well as processing techniques can no longer be used. In addition, the growth windows in epitaxy have to be modified in order to enhance vertical growth rates and reduce planar growth rates. Quite often, this leads to growth modes, which are far away from the ones regularly used for high efficiency planar LEDs. This talk will give an overview on the state of the art of our 3D GaN research, particularly focusing on MOCVD growth and 3D characterization. Potential advantages and challenges of this exciting new strategy towards low cost high efficiency solid state lighting will also be discussed.

DS 15: Organic Electronics and Photovoltaics II (jointly with CPP, HL, O)

Time: Tuesday 9:30–12:45 Location: H32

DS 15.1 Tue 9:30 H32

Influence of triplet excitons on the lifetime of polymer based organic light emitting diodes — •Oili Pekkola, Andrea Gassmann, Christian Melzer, and Heinz von Seggern — Electronic Materials Division, Institute of Materials Science, Technische Universität Darmstadt, Petersenstr. 23, 64287 Darmstadt, Germany

Despite the promising development of polymer based organic light emitting diodes (PLEDs), device lifetime and stability are still among the most critical issues. One of the lifetime-related factors investigated to a lesser extent is the influence of the high density of non-emissive triplet excitons which could be responsible for local heating or act as traps for charge carriers, leading to a degradation of the device.

This study utilizes PLEDs based on poly(p-phenylene vinylene) (PPV) derivatives to understand the influence of triplet excitons on the fatigue by increasing their amount in the PPV film. This increase is achieved by blending different concentrations of the triplet sensitizer platinum (II) octaethylporphine ketone (PtOEPK) into the PPV matrix in order to convert PPV singlet excitons to triplets. One observes that in PLEDs both the t50 and t90 lifetimes are drastically shortened in the presence of PtOEPK. To rule out a possible influence of the sole presence of PtOEPK on charge carrier transport, single carrier devices with different sensitizer contents were prepared. In these devices, no fatigue is observed regardless of the sensitizer concentration, suggesting that the decrease in the lifetimes of the bipolar diodes is indeed caused by the increased triplet population in the diodes with sensitized polymer films and not by the sensitizer additive as such.

DS 15.2 Tue 9:45 H32

Homogeneity of thin ZnTPP-films on silicon measured with reflectance anisotropy spectroscopy and Raman spectroscopy — •Stephan Peter Kate[1], Simona Pop[1], Jörg Rappich[2], and Karsten Hinrichs[1] — [1]Leibniz-Institut für Analytische Wissenschaften - ISAS - e.V., Albert-Einstein Str. 9, Berlin, 12489 Germany — [2]Helmholtz-Zentrum for Materials and Energy GmbH, Kekulestraße 5, Berlin, 12489, Germany

Organic devices for electronic applications are an important field of research. To improve the efficiency of those components, the analysis of structure and homogeneity of thin films is of crucial importance. In this study we demonstrate that Reflectance Anisotropy Spectroscopy (RAS) and Raman spectroscopy are useful to investigate the homogeneity of thin films of zinc-tetra-phenyl-porphyrin (ZnTPP) on silicon substrates. The RAS spectra of the thin films show an optical anisotropy in the visible spectral range. Analyzing the anisotropy, conclusions about the homogeneity of the thin films can be drawn. The vibrational modes of the molecules seen with resonant Raman spectroscopy are sensitive to the film structure. A pyrrole-bending mode in the region of 1075 cm-1 serves us as a marker for the film homogeneity. The RAS and Raman results are correlated with AFM measurements.

DS 15.3 Tue 10:00 H32

Morphology evolution of diblock copolymer based ZnO nanostructures upon solvent vapor treatment — •Kuhu Sarkar, Christoph Schaffer, Anna Naumann, Daniel Mosegui Gonzalez, and Peter Müller-Buschbaum — TU München, Physik Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching, Germany

Nanostructured inorganic metal oxides with tunable morphologies are desirable for optimizing many potential applications in the field of gas/chemical sensing, catalysis and energy storage. Zinc oxide (ZnO) is chosen in the present study owing to its outstanding optical and electrical properties. Different ZnO nanostructures are synthesized using a suitable diblock copolymer template via sol-gel chemistry. Zinc acetate dihydrate is used as the suitable commercial precursor for ZnO. There are several possibilities to tune the morphology as most of the diblock copolymers respond to the external fields such as temperature and solvent vapor. Hence, tetrahydrofuran solvent vapor treatment has been employed to the as-prepared thin films corresponding a grid-like morphology for different annealing times. Grazing incidence small angle X-ray scattering (GISAXS) has been performed to probe the structural order over the entire film volume. Evolution of the morphology has been followed by GISAXS studies as a function of different solvent treatment times. The annealed films are subsequently calcined at a higher temperature in order to understand the preservation of higher orders in the ZnO structure even after removal of the diblock copolymer.

DS 15.4 Tue 10:15 H32

Correlation of morphology and electronic properties of MoO_3 doped CBP layers I: TEM and electrical properties — •Daniela Donhauser[1,2], Levin Dieterle[1,2], Paul Heimel[3,2], Tobias Glaser[3,2], Maybritt Kühn[4,2], Mustapha Al-Helwi[5,2], Rasmus R. Schröder[6], Eric Mankel[4,2], Michael Kröger[1,2], and Wolfgang Kowalsky[1,2] — [1]Institut für Hochfrequenztechnik, TU Braunschweig, Braunschweig — [2]InnovationLab GmbH, Heidelberg — [3]Kirchhoff-Institut für Physik, Universität Heidelberg, Heidelberg — [4]Institut für Materialwissenschaft, TU Darmstadt, Darmstadt — [5]BASF SE, Ludwigshafen — [6]CellNetworks, Universität Heidelberg

Since electrochemical doping can significantly improve the performance of organic devices, the understanding of the fundamental properties of doped thin films is crucial. For a variety of different material systems a very low doping efficiency was observed, although from energetical considerations a very efficient charge transfer is expected. Using bright-field TEM and electron tomography we show for MoO_3-doped CBP ((4,4'-Bis(N-carbazolyl)-1,1'-biphenyl) thin films that this low doping efficiency is due to filament-like dopant agglomeration which can be controlled by changing the substrate temperature during the evaporation process [1]. The observed morphology is finally correlated with electrical properties like charge carrier density and mobility and depending on the dopant concentration an anisotropic charge transport is observed.

[1] Donhauser et al., Adv. Funct. Mater., 2012, 10.1002/adfm.201202089

DS 15.5 Tue 10:30 H32

Correlation of morphology and electronic properties of MoO_3-doped CBP layers II: IR spectroscopic study — •Tobias Glaser[1,5], Sebastian Beck[1,5], Daniela Donhauser[2,5], Maybritt Kühn[3,5], Bernd Lunkenheimer[4,5], Andreas Köhn[4,5], Eric Mankel[3,5], and Annemarie Pucci[1,5] — [1]Universität Heidelberg, Kirchhoff-Institut für Physik — [2]Technische Universität Braunschweig, Institut für Hochfrequenztechnik — [3]Technische Universität Darmstadt, Fachbereich Materialwissenschaft, Fachgebiet Oberflächenforschung — [4]Universität Mainz, Institut für Physikalische Chemie — [5]InnovationLab GmbH, Heidelberg

In order to obtain a further understanding on the charge transfer process in p-type doping using transition metal oxides, we performed insitu FTIR-spectroscopy on thin layers of 4,4'-Bis(N-carbazolyl)-1,1'-biphenyl (CBP) doped with MoO_3. In the doped layers, charge transfer complexes (CTCs) are formed, that exhibit a broad electronic excitation in the near IR region. These CTCs are located at the interface of the MoO_3 agglomerates and the organic matrix, inducing an interface dipole. The intensity of this electronic excitation in the spectra of layers with various doping concentrations indicates a linear increase of the agglomerates' surface area with MoO_3 concentration. The vibrational changes in the spectra of the doped layers indicate a charge transfer of Z=1e within the CTCs. By cooling the substrate during the deposition process, the agglomeration of the dopants can be suppressed.

Financial support by BMBF (project MESOMERIE) is gratefully acknowledged.

DS 15.6 Tue 10:45 H32

Correlation of morphology and electronic properties of MoO_3-doped CBP layers III: XPS and UPS study — •Maybritt Kühn[1,4], Eric Mankel[1,4], Daniela Donhauser[2,4], Tobias Glaser[3,4], Thomas Mayer[1,4], and Wolfram Jaegermann[1,4] — [1]Technische Universität Darmstadt, Fachgebiet Materialwissenschaft — [2]Technische Universität Braunschweig, Institut für Hochfrequenztechnik — [3]Universität Heidelberg, Kirchhoff-Institut für Physik — [4]InnovationLab GmbH, Heidelberg

Electro-chemical doping is a prerequisite to improve efficiency and conductivity of organic OLED materials. Here the p-type doping behavior of MoO_3 is analyzed using photoelectron spectroscopy (XPS/UPS). The doped CBP layers were evaporated and analyzed under UHV conditions. Concerning the Fermi level shift three different regimes can be distinguished: At low doping concentrations ($< 9\,$mol%) a rapid shift towards the HOMO level of CBP can be observed, becoming less strong and finally saturating at a maximum shift of 1 eV at a doping concentration of 45 mol%. The electron transfer from CBP to MoO_3 leads to the formation of reduced MoO_3. Determining the amount of these species we get information of the surface to volume ratio of the MoO_3 clusters in dependence of the doping concentration. Also here three different regimes can be distinguished. The morphology and Fermi level shift regimes will be correlated discussing the dopant morphology as shown in Talk I. Finally the amount of transferred charges is calculated regarding the reduced MoO_3 species and is compared with the number of cations determined by IR-spectroscopy (Talk II).

Coffee break (15 min)

DS 15.7 Tue 11:15 H32

Organic semiconductor devices on fibre shaped structures for smart textile applications. — •Tobias Könyves-Toth, Andrea Gassmann, and Heinz von Seggern — Electronic Materials Department, Institute of Materials Science, Technische Universität Darmstadt, Petersenstraße 23, 64287 Darmstadt, Germany

In the development of smart textiles already realized prototypes utilize embedded LEDs, displays or interactive communication devices based on inorganic semiconductor technology. Yet, these wearable smart textiles are not always comfortable since inorganic devices are stiff and rigid. On the other hand, organic electronic devices can be realized on flexible substrates employing very thin active layers of only about 100 nm thickness. The aim of the present work is to process organic semiconductor based devices directly on fibre surfaces. This task is challenging as manufacturing related problems due to the cylindrical shape of the fibre substrates and their small diameter of about 200 nm have to be overcome. Here, we present our findings on functional OLEDs on fibre substrates. Also the choice of proper fibre materials, ways to acquire smooth fibre surfaces and the structuring and encapsulation of fibre-shaped devices will be discussed. Additionally, methods to characterize the functionality of the devices, like angle dependence emission, will be presented.

DS 15.8 Tue 11:30 H32

Doping of organic semiconductors in case of dopant precipitation: the internal interface charge transfer doping model — •Thomas Mayer[1,2], Eric Mankel[1,2], Corinna Hein[1], and Wolfram Jaegermann[1,2] — [1]Technische Universität Darmstadt, Institute of Materials Science, Surface Science Division — [2]Innovation Lab Heidelberg

Doping of organic semiconductors is of paramount interest for device optimization as in addition to improved conductivity, engineering of space charge regions at interfaces e.g. of donor acceptor heterojunction solar cells is achieved. Photoemission data taken at the synchrotron BESSY on co-sublimed and bilayer films of prototypical organic semiconductors as CuPc and spiro-MeoTAD and prototypical p-type organic and inorganic dopants as TCNQ and WO3 show similar electronic trends, which can be explained assuming phase separation of the dopants within the matrix material. For metal oxides the precipitation is directly observed using TEM. For the doping induced variations of the matrix Fermi level in such semiconductor-dopant composites we propose the internal interface charge transfer doping model. According to this model the doping limit can be predicted from pristine matrix and pristine dopant electronic band diagrams. The model also admits of deriving measures that can be taken to improve doping efficiency.

DS 15.9 Tue 11:45 H32

Molecular orientation at heterojunctions for organic photovoltaics studied by NEXAFS — •Andreas Opitz[1], Norbert Koch[1], Ulrich Hörmann[2], Wolfgang Brütting[2], Christopher Lorch[3], Alexander Hinderhofer[3], Frank Schreiber[3], and Ellen Moons[4] — [1]Inst. f. Physik, Humboldt-Universität zu Berlin, Germany — [2]Inst. of Physics, University of Augsburg, Germany — [3]Inst. of Applied Physics, University of Tübingen, Germany — [4]Dept. of Physics and Electrical Engineering, Karlstad University, Sweden

Organic/organic heterojunctions are widely used in organic photovoltaic cells. The morphology at the interface, where the charge carrier separation takes place, plays an important role. In this contribution the interfaces between sexithiophene (6T) as donor and the acceptor materials fullerene (C_{60}) and diindenoperylene (DIP) [1] were analysed by angle resolved near-edge X-ray absorption fine structure spectroscopy and the results were compared to X-ray scattering data.

Different orientations are observed for molecules in the bulk, at free surfaces and at buried interfaces. Here, the orientation at the free surfaces depends on the substrate temperature during deposition for 6T but not for DIP. Furthermore, the acceptor molecules influence the orientation of the underlying 6T molecules. An improved crystallization and pronounced upright standing of the molecules in the underlying 6T film was observed upon deposition of C_{60}. In contrast the deposition of DIP on top of 6T leads to an orientational relaxation of the 6T molecules to the bulk inclination angle.

[1] U. Hörmann et al., phys. stat. sol. RRL 5 (2011) 241.

DS 15.10 Tue 12:00 H32

Electronic interface properties of PCBM using photoelectron spectroscopy — •Julia Maibach[1,2], Eric Mankel[1,2], Thomas Mayer[1,2], and Wolfram Jaegermann[1,2] — [1]Technische Universität Darmstadt, Fachbereich Materialwissenschaft — [2]InnovationLab GmbH, Heidelberg

The electronic interface properties of wet processed organic materials are of current interest as many fabrication techniques for organic electronic devices are based on inks. Photoelectron spectroscopy (PES) has proven to be a powerful method to investigate the electronic structure at semiconductor contacts. Due to high surface sensitivity of PES, the interface is generally prepared step by step in UHV. For films deposited from solution we integrated a newly developed ultrasonic nebulizer unit to the UHV cluster-tool of the analytic competence center at the InnovationLab, Heidelberg. Dilute solutions of Phenyl-C61-butyric acid methyl ester (PCBM) in Chlorobenzene were used to deposit the material on ozone and polymer treated ITO as well as on gold to investigate the contact behavior of PCBM. With the nebulizer method layer thicknesses in the range of 10-20 Å can be achieved while repeated exposure to the nebulae increased step by step the emission intensities of the PCBM. Furthermore drop-casting of thicker layers has been performed allowing in combination the thickness dependent determination of the electronic properties. In case of PCBM on ozone treated ITO the HOMO spectra shift 0.4 eV to higher binding energy with increasing thickness, indicating the formation of a space charge region in PCBM due to electron transfer from ozone treated ITO.

DS 15.11 Tue 12:15 H32

Carbon Nanotubes and Organic Solar Cells — •Gerhard Lackner[1], Richard Boucher[2], Vladimir Shvartsmann[1], Viktor Bezugly[2], Ingolf Endler[3], Mario Krug[3], Frank Meissner[3], Martin Mkandawire[4], and Doru C. Lupascu[1] — [1]Universität Duisburg-Essen, Essen, Germany — [2]Technische Universität Dresden, Dresden, Germany — [3]Fraunhofer-Institut für Keramische Technologien und Systeme IKTS, Dresden, Germany — [4]Verschuren Centre for Sustainabilty in Energy and the Environment, Cape Breton University, Canada

Materials like carbon nanotubes (CNT) attracted much attention by researchers all around the world due to their exceptional electrical, mechanical and chemical properties. Especially single-walled carbon nanotubes (SW-CNT) offer great opportunities in the field of new electrical devices, for instance field effect transistors based on their semiconductor properties. CNT are also used in organic photovoltaics (OPV) as acceptor material, to enhance charge carrier transport within organic layers or as transparent electrodes. The application of CNT as acceptor material and for charge carrier enhancement is the main topic of this work. Therefore, we studied the photovoltaic device performance of different material combinations of CNT, regio regular Poly(3-Hexylthiophen-2,5-diyl) (rr-P3HT), Phenyl-C61-butric acid methyl ester (PCBM) and copper phthalocyanine (CuPc). Furthermore, different device architectures were investigated and compared with each other.

DS 15.12 Tue 12:30 H32

n-channel percolation in a pentacene-C60 ambipolar organic thin film transistor — Simon Noever, Stefan Fischer, and •Bert Nickel — Ludwig-Maximilians-Universität, Fakultät für Physik & CENS, München, D

We present [1] a well balanced ambipolar organic field effect transistor with high hole and electron saturation mobilities of 0.28 cm*/Vs and 0.18 cm*/Vs, respectively. The structure and morphology of the respective films are analyzed using AFM and GIXS methods. Furthermore, we track the formation of a pentacene-C60 heterojunction by in-situ measurements during deposition of C60. Upon percolation of the n-channel, the heterojunction charges, acting as an additional top gate for the hole conducting channel. The fact that the p-channel threshold does not shift before the n-channel develops highlights two interesting findings for bilayer ambipolar TFTs. Apparently, before the C60 film percolates, the fullerene islands are electronically floating and the charging of the interface is confined to the pentacene-C60 contact area. Secondly, the threshold voltage shift of the p-channel upon fullerene percolation implicates the generation of a second hole conducting channel at the pentacene top surface. The introduced method demonstrates a way to evaluate the electrostatic situation in operating organic heterojunction devices. [1] S. Noever, S. Fischer, B. Nickel, Advanced Materials (in press)

DS 16: Organic Thin Films I

Time: Tuesday 14:45–16:15 Location: H32

DS 16.1 Tue 14:45 H32

Finite size effects in the excitonic line-shape of 2D ordered molecular aggregates — •Alexander Eisfeld[1], Mathias Müller[2], and Moritz Sokolowski[2] — [1]MPI-PKS Dresden — [2]Institut für Physikalische und Theoretische Chemie der Universität Bonn, Wegelerstrasse 12, 53115 Bonn, Germany

We consider molecules that are regularly arranged in a two-dimensional layer. The molecules can exchange excitation energy via transition-dipole-dipole interaction, which leads to the formation of a exciton-band. The arrangement is such that a J-aggregate is formed, i.e. the dominant absorption is red-shifted with respect to the non-interacting molecules.

Usually the absorption line-shape of the J-aggregate is much narrower then that of the individual monomers. Recent experiments on PTCDA molecules on a KCl surface showed an absorption line-shape that is considerable broadened. We will discuss possible mechanisms responsible for this broadening.

DS 16.2 Tue 15:00 H32

Electronic and Geometric Structure of PTCDI-C13 Molecules on SAM Modified Noble Metal Surfaces — •Daniel Gebauer[1], Philip Schulz[2], Tobias Schäfer[1], Domink Meyer[1], Ingolf Segger[1], Carolin Jacobi[1], Christian Effertz[1], and Matthias Wuttig[1] — [1]I. Inst. of Physics (IA), RWTH Aachen Univ. — [2]Dept. of Elect. Engineering, Princeton Univ.

The molecule N,N'-Ditridecylperylene-3,4,9,10-tetracarboxylic diimide (PTCDIC-13) is a promising semiconductor for organic thin film transistors (TFTs). It is well known that the interfacial design is one crucial aspect of device tuning. We have shown before that the modification of electrodes with dithiocarbamate (DTC) self-assembling monolayers leads to a significantly enhanced transistor performance [1]. To gain a deeper understanding of this mechanism we have performed an investigation at the interface of PTCDI-C13 and noble metal surfaces, which are modified by DTCs. Therefore we have prepared thermally evaporated, ultra-flat samples with (111)-orientation of noble metals on mica and subsequently deposited PTCDI-C13 monolayers on the metals with and without SAM-modification. The energy level alignment between the PTCDI-C13 and the DTC modified metal surfaces has been determined by Ultraviolet Photoelectron Spectroscopy (UPS), while the chemical binding is investigated by X-ray Photoelectron Spectroscopy (XPS). The molecular orientations of the molecules are analyzed by Fourier Transform Infrared Spectroscopy (FTIR).

[1] P. Schulz et al., 2011 MRS Fall Meeting U13.17

DS 16.3 Tue 15:15 H32

Spectroscopy on N-Type Doped Manganese Phthalocyanine — •Michael Ludemann[1], Francisc Haidu[1], Philipp Schäfer[1], Benjamin Mahns[2], Daniel Lehmann[1], Ovidiu D. Gordan[1], Jens Kortus[3], Martin Knupfer[2], and Dietrich R.T. Zahn[1] — [1]TU Chemnitz, 09126 Chemnitz, Germany — [2]IFW Dresden, 01069 Dresden, Germany — [3]TU BA Freiberg, 09596 Freiberg, Germany

In the fabrication processes of organic semiconductor devices, n-type doping of organic thin films still remains challenging. Intercalated alkali metals act as electron donors and thus increase the electrical conductivity of transition metal phthalocyanines [1]. In this study, manganese phthalocyanine (MnPc) thin films (5–100 nm) are prepared by organic molecular beam deposition (OMBD) under ultra-high vacuum (UHV) conditions. Doping is achieved via subsequent potassium (K) evaporation afterwards. Electron energy loss spectroscopy (EELS) [2] and *in situ* spectroscopic ellipsometry (SE) reveal that the optical properties of MnPc change dramatically during K doping. Finally, *in situ* online monitoring of the vibrational properties provides deep insight into the doping dynamics. In this work, the results obtained by EELS, SE, and Raman spectroscopy are compared, showing a formation of consecutive potassium doped MnPc phases with distinct optical and vibrational properties.

[1] M. F. Craciun *et al.* J. Am. Chem. Soc. **127** (2005) 12210

[2] B. Mahns *et al.* J. Chem. Phys. **134** (2011) 194504

DS 16.4 Tue 15:30 H32

Changes in glassy polymers induced by light — •Ioan Botiz[1,2], Paul Freyberg[1], Natalie Stingelin[3], Arnold Chang-Mou Yang[4], and Günter Reiter[1,2] — [1]Institute of Physics, University of Freiburg, Freiburg, Germany — [2]Freiburg Institute for Advanced Studies, Freiburg, Germany — [3]Imperial College London, London, UK — [4]National Tsing Hua University, Hsinchu, Taiwan

We have experimentally compared the photoluminescence (PL) emission from a thin film of conjugated poly[2-methoxy-5-((2'-ethylhexyl)oxy)-1,4-phenylenvinylene] (MEH-PPV) embedded in a polystyrene (PS) inert matrix, with and without exposure to light. A systematic variation of temperature, conjugated polymer content in the PS inert matrix and film thickness revealed an increase of PL of up to 30% for films exposed to light of wavelength shorter than 700 nm. The increase in PL was higher for thinner films containing 100% MEH-PPV and kept at 35 °C (at this temperature both MEH-PPV and PS are glassy) during 1 hour of illumination. All experiments were performed under nitrogen atmosphere. We tentatively propose that this enhancement of PL is due to changes in conformation induced even in the glassy state of conjugated molecules trough photoexcitations. Deformation of conjugated molecules by light might lead to a reduced phonon-exciton coupling of these polymer chains, i.e. to better PL emission.

DS 16.5 Tue 15:45 H32

Encapsulated metal nanoparticles for absorption enhancement of thin film organic photovoltaic cells — •Verena Kolb[1,2], Andreas Steindamm[1,3], Michael Brendel[1,3], Martin Kamp[4], and Jens Pflaum[1,3] — [1]Experimental Physics VI, Julius Maximilians University of Würzburg, 97074 Würzburg — [2]Center for Nanosystems Chemistry, 97074 Würzburg — [3]ZAE Bayern, 97074 Würzburg — [4]Technical Physics, Julius Maximilians University of Würzburg, 97074 Würzburg

Utilization of plasmonic effects at metal nanoparticle surfaces provides an interesting approach to modify the optical properties of molecular thin films and thereby, to enhance their effective absorption. This enhancement is caused by an increase of the near-field component and the scattering of incident light and might be applied in e.g. organic photovoltaic (OPV) cells. However, as a drawback such metal particles are able to quench the photogenerated excitons and trap free charges. An encapsulation of the particles may help to reduce these loss mechanisms. In this contribution we present our latest results on preparation of encapsulated metal particles and their influence on thin layers of the organic semiconductor Diindenoperylene (DIP). Optical effects are measured via UV/VIS and photoluminescence spectroscopy. Finally DIP/C_{60} OPV cells with embedded particles were built and electrically and optically characterized. Financial support by the Solar Technologies go Hybrid project is gratefully acknowledged.

DS 16.6 Tue 16:00 H32

Effect of fluorination: Optical properties of Rubrene in films and solution — •Falk Anger[1], Reinhard Scholz[2], Evelyn Adamski[1], Katharina Broch[1], Alexander Gerlach[1], Yoichi Sakamoto[3], Toshiyasu Suzuki[3], and Frank Schreiber[1] — [1]Institut für Angewandte Physik, Auf der Morgenstelle 10, 72076 Tübingen — [2]Institut für Angewandte Photophysik, TU Dresden, 01069 Dresden — [3]Institute for Molecular Science, Myodaiji, Okazaki 444-8787, Japan

A promising way to modify the electronic levels of organic semiconductors is partial or complete fluorination, potentially with further opportunities opening up by mixing these compounds with the hydrogenated version [1]. We present the optical properties of newly synthesised fully ($C_{42}F_{28}$) and half-fluorinated ($C_{42}F_{14}H_{14}$) rubrene, both in thin films and as monomers in solution, and compare them to hydrogenated rubrene ($C_{42}H_{28}$, RUB) [2]. Remarkably, all three compounds show similar optical absorption bands and photoluminescence line shapes. The results are interpreted with density functional calculations of the orbital energies and time-dependent density functional theory for the HOMO-LUMO transition [3]. Red shifts induced by the surrounding solvent or organic thin films remain much smaller than for polyacenes, in keeping with previous observations for rubrene and existing models for the solvatochromic shifts. We discuss implications for applications of the new material.

DS 17: Focus Session: Thin Film Photovoltaic Materials and Solar Cells I

Thin film photovoltaics based on inorganic materials such as Si, CdTe and chalcopyrites has received much attention during the last decades, yielding good progress in the understanding of the physical properties and device physics of these materials and solar cell structures, although there are still many open questions remaining. Currently there is much interest in expanding the photovoltaic materials spectrum to include earth abundant and nontoxic elements, with high absorption coefficients, tunable band gaps, large charge carrier mobilities and low defect densities, and also to explore nanostructure configurations. This focused session is intended to highlight some of the state-of-the-art research and challenges encountered in thin film photovoltaics using different materials, and also to bring in views from related energy research areas such as thermoelectrics and photoelectrochemical water splitting, which are on first sight distinct topics, but in fact share many commonalities. (Organizer: Thomas Unold, Helmholtz-Zentrum Berlin)

Time: Wednesday 9:30–12:45 Location: H32

Invited Talk DS 17.1 Wed 9:30 H32

Meso-Superstructured Perovskite Solar Cells — •Henry J. Snaith — University of Oxford, Parks Road, Oxford, OX13PU, UK

Combining both ultimately low cost materials and production with a high efficiency solar technology has thus far been elusive. Low cost materials, such as organics and oxides, tend to suffer from fundamental energy losses required to separate excitons and collect free charge carriers in electronically disordered semiconductors. For organic and dye-sensitized solar cells this energy loss, defined as the difference between the optical band gap and the open-circuit voltage, is typically 0.65 to 0.8 eV, but for a "perfect" single junction solar cell the theoretical minimum losses, as determined by the Shockley Quasar limit are in the region of 0.25 eV. Here I will present a new hybrid solar cell concept based on a printable mesoporous superstructured perovskite absorber combined with an organic hole conductor, which we term a "meso-superstructured solar cell" (MSSC). The minimal fundamental losses are as small as 0.45 eV, and the full sun power conversion efficiency is in excess of 10% in a single junction device. I will describe the concept, operating principles, recent progress.

Invited Talk DS 17.2 Wed 10:00 H32

Thermoelectric perovskite-type oxides and Heusler phases — •Anke Weidenkaff[1,2], Sascha Populoh[1], Leyre Sagarna[2], Gesine Saucke[1], Andrey Shkabko[1], and Nina Vogel[1] — [1]Empa — [2]Uni Bern

Solar energy can be converted by photovoltaic and photocatalytic processes or by high temperature conversions using concentrated solar radiation. Metal oxides and oxynitrides with perovskite-type structure show substantial potential for thermoelectric conversion processes using concentrated solar radiation as power source. Dense and highly nanostructured thin films are produced by chimie douce [1] and plasma methods [2]. Compositions and morphologies are changed in order to tune the band structure and defects. The thin films provide an alternative way to receive suitable samples to determine the phonon and charge carrier transport and thermoelectric properties. Advanced analytical tools are applied to unravel the structure-property relationships. References [1] Alfaruq, Dimas S., Otal, Eugenio H, Aguirre, Myriam H., Populoh, Sascha, Weidenkaff, Anke, Thermoelectric properties of CaMnO3 coatings and thin films obtained by soft chemistry synthesis routes, Journal of Materials Research, 27, (2012) 985-990. [2] Vogel-Schäuble, N., Romanyuk, Y.E., Yoon, S., Saji, K.J., Populoh, S., Pokrant, S., Aguirre, M.H., Weidenkaff, A., Thermoelectric properties of nanostructured Al-substituted ZnO thin films, Thin Sold Films, 520 (2012) 6869-6875

Topical Talk DS 17.3 Wed 10:30 H32

Photoelectrochemical Water Splitting with Complex Metal Oxides: the Role of Defects — •Roel van de Krol — Institute for Solar Fuels, Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany

Transition metal oxides are promising candidates for the conversion of solar energy to chemical fuels. They combine reasonable semiconducting properties with excellent chemical stability and low cost. As such, they can bridge the gap between conventional PV semiconductors and molecular/biological systems. Although exciting progress has been made in the past 5 years on e.g. Fe2O3 and Cu2O, further improvement of these binary oxides is severely hampered by intrinsic materials limitations. To broaden the scope of suitable materials, research efforts are currently shifting towards multinary (complex) oxides such as InVO4 and BiVO4. In InVO4, ionic point defects are found to enhance the visible light absorption, but they also cause extensive recombination. In contrast, BiVO4 is found to be a much more defect-tolerant material, showing internal QEs above 90% when prepared with a low-cost spray pyrolysis technique. We will discuss how photo-electrochemical measurements can be used to determine the performance-limiting factors in this material. This provide valuable guidelines to improve the photoresponse, resulting in a stand-alone water splitting device based on a BiVO4 photoanode and a thin film double-junction a-Si cell with a solar-to-hydrogen efficiency of 4.3%.

Coffee break (15 min)

Topical Talk DS 17.4 Wed 11:15 H32

Intrinsic point defects in CuInSe$_2$ and CuGaSe$_2$ studied by screened-exchange hybrid density functional theory — •Karsten Albe und Johan Pohl — TU Darmstadt, Insititut für Materialwissenschaft, FG Materialmodellierung, Petersenstr. 32, D-64287 Darmstadt

Cu(In,Ga)Se$_2$ is one of the most promising absorber material for solar cells. However, the presence of intrinsic point defects can be detrimental to the device properties, because of intrinsic doping and the formation of trap levels. These may act as recombination centres and therefore limit the device efficiency. Therefore, an in-depth understanding of the role of point defects in these devices is essential for optimizing the solar cell efficiency. In this talk, we discuss all relevant intrinsic point defects in terms of their defect formation energies, their charge transition levels and their localized single-particle states in the band gap, where applicable. First, the role of copper vacancies and interstitials for copper diffusion and Fermi-level pinning in the material will be discussed. Then Cu$_{\mathrm{In}}$ and Cu$_{\mathrm{Ga}}$ antisites are investigated and identified as hole traps with two distinct levels within the band gap, one of which can be attributed to the experimentally observed N2 level. Ga$_{\mathrm{Cu}}$ is confirmed as a deep defect in CuGaSe$_2$ and complex formation of antisites with copper vacancies is found not to be decisive for explaining the favourable properties of CuInSe$_2$, since In$_{\mathrm{Cu}}$ is already shallow by itself. The results also raise doubts about the relevance of selenium vacancies and DX centers for experimentally observed metastabilities.

Topical Talk DS 17.5 Wed 11:45 H32

Energy Band Alignment in Thin Film Solar Cells — •Andreas Klein — Technische Universität Darmstadt, Institut für Materialwissenschaft

The energy band alignment at interfaces between covalently bonded semiconductors like Si and GaAs can be well described using the charge neutrality level concept. The electrostatic potential distribution across an interface of such materials can be directly obtained once the band alignment and the doping profiles are known. In contrast to such ideal semiconductor interfaces, thin film solar cells employ more ionic compounds, combination of dissimilar materials, and (low temperature) film deposition techniques being far from equilibrium. As a consequence, deposited films may contain a high concentration of defects, which can prevent a variation of the Fermi energy. Such a bulk Fermi level pinning limits the evolution of band bending at an interface and can even lead to a large variation of energy band alignment. These effects may be a natural explanation for the sensitivity of solar cell efficiency on the selection of material combinations and deposition techniques and therefore enable new optimization strategies. It further suggests that simulation of electrical cell characteristics assuming ideal semiconductor behaviour may not be adequate.

Topical Talk DS 17.6 Wed 12:15 H32

Nanowire device concepts for thin film photovoltaics — •Silke Christiansen — Max-Planck-Institute for the Science of Light, Erlangen, Germany — Institut of Photonic Technology, Jena, Germany

Large-area aligned SiNW arrays are fabricated on Si wafers and multicrystalline layers on glass substrates via metal-catalyzed wet chemical etching (WCE) or dry etching processes with or without prior lithographic patterning the use of densely packed well organized polystyrene (PS) spheres as a mask. The diameter, length, packing density, and even the shape of SiNWs could precisely be controlled and tuned by adjusting either plasma etching duration or chemical etching conditions and the diameter and pitch of the PS spheres. The anti-reflective properties of SiNWs and thus the extremely high absorption in thin SiNW layers are essential for NW based next generation solar cells. Several cell concepts with SiNWs are realized including most interesting ones: a hybrid organic/inorganic solar cell using SiNWs as absorber and PEDOT:PSS as a conducting polymer, a semiconductor-insulator-semiconductor (SIS) cell concept with SiNWs as absorbers and a tunneling barrier for charge carrier separation. The thin tunneling oxide is Al2O3 with a thickness of only a few Å and a transparent conductive oxide (TCO here: Al:ZnO) are both grown conformally around the SiNWs using atomic layer deposition (ALD).The first solar cell prototypes of 1-2cm2 area on glass substrates reached (i) open-circuit voltage of 625 mV, a short-circuit current density of 20 mA/cm2 and efficiencies >7% and (ii) an open-circuit voltage of 550 mV, a short-circuit current density of 33 mA/cm2 and efficiencies >10%.

DS 18: Micro- and Nanopatterning (jointly with O)

Time: Wednesday 9:30–11:30 Location: H8

DS 18.1 Wed 9:30 H8

Evolution of Ge surface topography during low energy ion beam erosion — •Marc Teichmann, Jan Lorbeer, Frank Frost, and Bernd Rauschenbach — Leibniz-Institut für Oberflächenmodifizierung e.V., Permoserstraße 15, 04318 Leipzig, Germany

The self-organized pattern formation on Ge(100) by low-energy ion beam sputtering with noble gases is studied. We investigated the surface topography in dependency on the angle of incidence. Furthermore the evolving structures are investigated as a function of ion beam energy in the range from 400 eV up to 2000 eV and in a fluence range form $1.1 \times 10^{18}\,\mathrm{cm}^2$ until $1.3 \times 10^{19}\,\mathrm{cm}^2$.

The surface remains flat up to an angle of incidence of about 60 deg before a ripple pattern evolves at higher angles with wave vector parallel to the projection of the ion beam. This pattern also vanishes at 75 deg when a saw tooth profile evolves on the surface. At grazing incidence a pattern emerges with wave vector perpendicular to the ion beam. Furthermore we observe an energy dependency on the transition between smoothening and patterning and a temporal coarsening of the structures. The observations suggest that the projectile mass is an important parameter for pattern formation and gradient dependent sputtering is a main mechanism of surface destabilization which is also supported by TRIM.SP [1] calculations that also reveal that reflected ions can contribute to surface stabilization and surface smoothing.

Support by Deutsche Forschungsgemeinschaft through FOR 845 is gratefully achknowledged.

[1] J. P. Biersack, W. Eckstein, Appl. Phys. A, **34**, 73-94 (1984).

DS 18.2 Wed 9:45 H8

Pattern formation on sapphire by low energy ion beam erosion — •Jan Lorbeer, Marc Teichmann, Frank Frost, and Bernd Rauschenbach — Leibniz Institut für Oberflächenmodifizierung e.V, Leipzig, Deutschland

The pattern formation on sapphire by low-energy ion beam erosion is investigated. In detail the influence of the ion incidence angle ($\theta = 0 - 85$ deg), ion energy ($E_{ion} = 400 - 2000$ eV), ion species (Ne, Ar, Kr, Xe) and fluence ($\Phi \approx 2 \times 10^{18} - 1.5 \times 10^{19}$ cm^{-2}) were evaluated.

In general there are four regimes of surface evolution. At low incidence angles the surface is smoothened with an minimal RMS value of about 90 pm. At angles of around 50 deg a ripple pattern develops. The wavelengths can be tuned in the range from 10 to 50 nm. Following the surface becomes faceted, connectet with a maximum in the surface roughness at about 75 degrees. At even higher incidence angles the surface is smoothened again.

It has been shown, that the regualarity of the formed ripples strongly depends on the ion mass, whereby heavier ions form a more regular surface pattern.

For higher ion energies the onset of ripple formation shifts to higher incidece angles.

Support by Deutsche Forschungsgemeinschaft through Forschergruppe 845 is gratefully acknowledged.

DS 18.3 Wed 10:00 H8

Modelling the etching behavior of GaAs irradiated with protons in a proton beam writing process — •Ulrich Vetter, Tristan Koppe, Charlotte Rothfuchs, and Hans Hofsäss — 2. Physikalisches Institut, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen

Creating three dimensional structures in semiconductors such as GaAs is a very promising application of proton beam writing [1] which has been realized recently without changing the beam energy or the ion species, but simply by varying the fluence during MeV proton irradiation [2]. In order to predict the evolving structures in the subsequent electrochemical etching process it is desirable predict the 3D damage concentration distribution as input for finite element simulations of the etching process. This distribution is determined from SRIM simulations [3] and the damage dependent transition behavior known from work on proton implantation isolation frequently applied in semiconductor manufacturing processes [4].

[1] J.A. van Kan et al., Appl. Phys. Lett. 83 (2003) 1629.

[2] M. Schulte-Borchers , U. Vetter, T. Koppe, H. Hofsäss, J. Micromech. Microeng. 22 (2012) 025011.

[3] J.F. Ziegler, J.P. Biersack, and M.D. Ziegler. SRIM - The Stopping and Range of Ions in Matter. SRIM Co. 2008.

[4] S.J. Pearton, Mater. Sci. Rep. 4 (1990) 313

DS 18.4 Wed 10:15 H8

Selective deposition of nanospheres in trenches on silicon surfaces by self-organisation — •Katharina Brassat and Jörg K. N. Lindner — University of Paderborn, Paderborn, Germany

The self-organisation of nanospheres on surfaces has been extensively studied in the last decades, as it allows for the simple and cost-effective creation of regular arrays of nano-objects such as metallic nanodots. These can be achieved by nanosphere lithography (NSL), i.e. deposition of a metal through a monolayer of nanospheres acting as a mask. Various techniques have been invented to create nanosphere monolayers as a first step of NSL. In the present work, we use the spreading knife technique as a fast and well controllable large area convective self-assembly technique in order to form chains of nanospheres sitting in a linear trench on a pre-patterned silicon surface. The goal is to use these templates as a deposition mask, by which linear chains of opposing metallic nanotips can be formed. Optical lithography and reactive ion etching (RIE) are used to form trenches on Si(100) wafers whose shape, depth and width are subsequently investigated by confocal laser scanning microscopy (CLSM). Using the spreading knife technique, polystyrene (PS) spheres with a diameter of 2.1 *m are assembled exclusively inside the trenches. This is achieved by optimisation of process parameters and functionalisation of the silicon surface with amphiphilic agent octadecyltrichlorsilane (OTS) which forms a self-assembled molecular monolayer (SAM). By this, linear chains of tangent PS-spheres with a length of up to 0.5 mm are obtained and can be used as a deposition mask.

DS 18.5 Wed 10:30 H8

Nickel Nanodot Arrays on Silicon formed by Nanosphere Lithography: A TEM Study — •Johannes Pauly and Jörg K. N. Lindner — Department of Physics, University of Paderborn, 33098 Paderborn, Germany

Nanosphere lithography (NSL) is a cost-effective bottom-up technique to form equally sized nanodots on surfaces, which can be easily scaled up to large areas. It is based on the self-organized arrangement of colloidal nanospheres in a hexagonally close packed monolayer which serves as a shadow mask for a subsequent thin film deposition process. The lateral size of nanodots and their density depend on the diameter of spheres, while the exact shape of dots depends on the deposition method and the dot/substrate combination used. This is due to the fact that the deposition technique defines the angular distribution of atoms arriving at the sample and the dot/substrate materials combination determines the crystallization and wetting properties of the dots. In addition the clogging of masks strongly affects the growth of dots. While in previous studies mostly scanning electron and atomic force microscopy were used to image dots, in the present study transmission electron microscopy is used to characterize the shape and structure of dots. To this end nanosphere masks of several square centimetre size were prepared on silicon using a doctor blade technique and an aqueous suspension of polystyrene spheres. Nickel thin films were deposited by thermal evaporation at room temperature. It is shown that nanocrystalline triangular Ni dots with extremely sharp tips are formed, the radius of tip curvature being given by the size of Ni grains.

DS 18.6 Wed 10:45 H8

Fabrication and electrical transport properties of binary Co-Si nanostructures prepared by focused electron beam-induced deposition — •Fabrizio Porrati and Michael Huth — Physikalisches Institut, Goethe Universität, Frankfurt am Main

CoSi-C binary alloys have been fabricated by focused electron beam-induced deposition (FEBID) by the simultaneous use of dicobaltoctacarbonyl, $Co_2(CO)_8$, and neopentasilane, Si_5H_{12}, as precursor gases. The alloys are made of Co-Si nanoparticles embedded in a carbonaceous matrix. By varying the relative precursors fluxes, alloys with variable Si:Co ratio are obtained. The electrical transport properties are governed by the electron tunneling between neighboring Co nanoparticles. According with the metal content of the alloy, the electrical conductivity can be tuned from the insulating regime into the quasi-metallic tunneling coupling regime.

DS 18.7 Wed 11:00 H8

Realizing three-dimensional nanostructures using nanotemplates: concept, properties and high performance devices — •Fabian Grote, Liaoyong Wen, Zhibing Zhan, Ahmed Al-Haddad, Yan Mi, Samar Tarish, Chengliang Wang, Ranjith Vellacheri, Huaping Zhao, and Yong Lei — Fachgebiet 3D-Nanostrukturierung, Institut für Physik & IMN MacroNano (ZIK), Technische Universität Ilmenau, Prof. Schmidt Str. 26, 98693 Ilmenau, Germany

Here we introduce a templates-based three-dimensional (3D) nanostructuring technique,[1,2] which has been utilized to fabricate diverse functional 3D nanostructures in our group, including highly ordered arrays of nanowires, nanotubes, core-shell and heterojunction nanowire and tubes. Due to the well-defined structures of nano-porous templates, the structural parameters of the prepared 3D nanostructures can be precisely controlled, such as size, length, spacing and tube thickness. The fabrication processes of the proposed 3D nano-structuring technique is highly cost-effective for preparing large-area of nanostructure arrays, which is desirable for device applications. So far different devices have been constructed based on these 3D nanostructures including supercapacitors, sensors, catalysts and solar cells. The high performance of these devices confirms that this innovative 3D nanostructuring technique is the key to realize the next generation of functional nano-devices. Reference: [1] Y. Lei, S. Yang, M. Wu, G. Wilde, Chem. Soc. Rev. 2011, 40, 1247. [2] Y. Lei, W. Cai, G. Wilde, Progress in Materials Science 2007, 52, 465.

DS 18.8 Wed 11:15 H8

Characterization of high-end photomasks by spectroscopic ellipsometry — •Anett Heinrich[1], Ingo Dirnstorfer[1], Thomas Mikolajick[1], Jörg Bischoff[2], and Uwe Richter[3] — [1]NaMLab gGmbH, 01187 Dresden, Germany — [2]Osires, 98693 Ilmenau, Germany — [3]Sentech Instruments GmbH, 12489 Berlin, Germany

We evaluated spectroscopic ellipsometry as an optical metrology method to determine critical parameters on nanostructured photomasks in high resolution and short process time. An industrial opaque MoSi on glass (OMOG) photomask with line/space gratings consisting of pitches between 280 and 640 nm and different duty cycles was analyzed. The polarization-dependent diffraction effects in Psi and Delta were measured in a wavelength range of 320 to 800 nm. The mask parameters were determined by modeling the ellipsometric response with the rigorous coupled wave analysis (RCWA) method. It was found that the pitch could be determined within sub-nm accuracy down to 130 nm, where the rayleigh singularities move out of the spectral range. The simulated critical dimension (CD) values are systematically smaller than the nominal mask CD. This CD offset was between 10 to 25 nm depending on the absolute CD. A through pitch sensitivity analysis showed that the evaluated metrology is sensitive to CD variations even for sub-50 nm features.

DS 19: Spin Effects in Molecules at Surfaces (jointly with MA, O)

Time: Wednesday 9:30–12:15 Location: H23

DS 19.1 Wed 9:30 H23

Weak Coupling Kondo Effect in a Purely Organic Molecule: Universal Temperature and Magnetic Field Dependence — •Markus Ternes[1], Steffen Kahle[1], Yung-hui Zhang[1], Tobias Herden[1], Uta Schlickum[1], Peter Wahl[1,2], and Klaus Kern[1,3] — [1]Max-Planck-Institute for Solid State Research, Heisenbergstr. 1, 70569 Stuttgart, Germany — [2]School of Physics and Astronomy, University of St. Andrews, North Haugh, St. Andrews, Scotland — [3]Institut de Physique de la Matière Condensée, Ecole Polytechnique Fédérale de Lausanne, 1015 Lausanne, Switzerland

The Kondo effect is one of the most intriguing any-particle phenomenon in solid-state physics due to the simplicity of the underlying model: the scattering of itinerant electrons at a localized spin.[1] It has been intensely studied on the single atomic and molecular level by scanning tunneling spectroscopy (STS) in the last two decades; however a quantitative comparison with theoretical predictions remained challenging due to orbital degeneracies and a spin quantum number higher than $\frac{1}{2}$. Here, we present STS measurements on an purely organic radical coupled to the conduction electrons of a Au(111) surface. The observed zero bias anomaly is due to a spin $\frac{1}{2}$ Kondo screening in the weak coupling limit. We can describe the temperature and magnetic field dependence of the spectral features practically parameter free by perturbation theory allowing quantitative tests on more complex theoretical models.
[1] A. C. Hewson, 1997: The Kondo Problem to Heavy Fermions, Cambridge University Press

DS 19.2 Wed 9:45 H23

Density Functional Investigation of a Phthalocyanine Based Spin Transfer Material — •Rico Friedrich[1], Susi Lindner[2], Torsten Hahn[1], Claudia Loose[1], Martin Knupfer[2], and Jens Kortus[1] — [1]TU Bergakademie Freiberg, Freiberg, Germany — [2]IFW Dresden, Dresden, Germany

Interfaces were found to be of outstanding importance for electronic and spin transfer purposes especially in molecular spintronics [1]. Recently it has been demonstrated that an organic interface purely made from metal phthalocyanines namely manganese phthalocyanine (MnPc) and perfluorinated cobalt phthalocyanine ($\mathrm{F}_{16}\mathrm{CoPc}$) exhibits a charge and spintransfer at the interface between both molecules [2]. In this talk we present a systematic theoretical investigation of the phthalocyanine based dimer $\mathrm{MnPc}^{\delta+}/\mathrm{F}_{16}\mathrm{CoPc}^{\delta-}$ within density functional theory framework. For all considered stackings a charge transfer from MnPc to $\mathrm{F}_{16}\mathrm{CoPc}$ is observed which outlines this behavior as an intrinsic property of the molecular pair. In addition a ferromagnetic coupling ($S = 2$) of the molecular magnetic moments within the dimer is always observed due to 90° superexchange and direct exchange contributions. The comparison of the calculated absorption spectra of the geometrical arrangements to the experimentally recorded electron energy-loss spectrum strongly indicates the β-geometry to be preferred over all others. Only for this geometry an experimentally observed excitation around 0.6 eV is reproduced by the calculation.
[1] S. Sanvito, Nature Physics **6**, 562, (2010).
[2] S. Lindner *et al.*, Phys. Rev. Lett. **109**, 027601, (2012).

DS 19.3 Wed 10:00 H23

Superexchange-mediated ferromagnetic coupling in two-dimensional Ni-TCNQ networks on metal surfaces — •Sebastian Stepanow[1], Nasiba Abdurakhmanova[1], Tzu-Chun Tseng[1], Alexander Langner[1], Christopher Kley[1], Violetta Sessi[2], and Klaus Kern[1,3] — [1]MPI-FKF Stuttgart — [2]ESRF Grenoble — [3]EPFL Lausanne

We investigate the magnetic coupling of Ni centers embedded in two-dimensional metal-coordination networks self-assembled from 7,7,8,8-Tetracyanoquinodimethane (TCNQ) molecules on Ag(100) and Au(111) surfaces. X-ray magnetic circular dichroism (XMCD) measurements show that single Ni adatom impurities assume a spin-quenched configuration on both surfaces, while Ni atoms coordinating to TCNQ ligands recover their magnetic moment and exhibit ferromagnetic coupling. The valence state and the ferromagnetic coupling strength of the Ni coordination centers depend crucially on the underlying substrate due to the different charge state of the TCNQ ligands on the two surfaces. The results suggest a superexchange coupling mechanism via the TCNQ ligands.

DS 19.4 Wed 10:15 H23

Interface magnetism of the phenalenyl based molecular dimer adsorbed on a ferromagnetic surface — •Nicolae Atodiresei, Vasile Caciuc, and Stefan Blügel — Peter Grünberg Institut (PGI-1) and Institute for Advanced Simulation (IAS-1), Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

Molecular based magnetic units represent a very exciting avenue in designing and building future data storage, sensing and computing multifunctional devices. The density functional theory (DFT) provides a framework that reliably describes the electronic properties of molecules adsorbed on magnetic surfaces which are an essential perquisite for the design an understanding of the functionality of hybrid organic molecular spintronic devices. We will present *ab initio* studies performed to understand the interaction of a phenalenyl (PLY) based molecular dimer with a ferromagnetic Co surface. Charge transfer and hybridization between the atomic p_z orbitals of the PLY with the $d-$orbitals of the Co atoms create new hybrid metal-organic interface states [1,2] that lead to a large interfacial magnetoresistance near room temperature as measured in experiments [3]. Furthermore, our studies demonstrate the decisive role played by the van der Waals interactions in correctly describing the interaction between aromatic PLY dimers and metallic surfaces.
[1] N. Atodiresei *et al.*, Phys. Rev. Lett. **105**, 066601 (2010).
[2] N. Atodiresei *et al.*, Phys. Rev. B **84**, 172402 (2011).
[3] K. V. Raman *et al.*, accepted for publication in Nature (2012).

DS 19.5 Wed 10:30 H23

Magnetism and molecule-surface interaction in transition metal porphyrin molecules on Cu(001) — •H. C. Herper[1,2], S. Bhandary[2], M. Bernien[3], C. F. Hermanns[3], A. Krüger[3], E. Weschke[4], C. Czekelius[5], C. Weis[1], C. Antoniak[1], B. Krumme[1], J. Miguel[3], D. Bovenschen[1], B. Sanyal[2], W. Kuch[3], H. Wende[1], and O. Eriksson[2] — [1]Fakultät für Physik und CeNIDE, Universität Duisburg-Essen, Germany — [2]Department of Physics and Astronomy, Uppsala University, Sweden — [3]Institut für Experimentalphysik, Freie Universität Berlin, Germany — [4]Helmholtz-Zentrum Berlin, Germany — [5]Institut für Chemie und Biochemie, Freie Universität Berlin, Germany

We present a combined theoretical and experimental study of Fe(Co) porphyrin molecules on (O)/Cu(001) surfaces. The interaction between nonmagnetic surfaces and molecules is weak, hence the anisotropy of the molecule can be studied together with the influence of ligands and hybridization effects with the surface. Magnetic and structural properties have been investigated within DFT and angle-dependent X-ray absorption spectroscopy at the Fe $L_{2,3}$ edge. The magnetic dipole term is calculated to allow for comparison between spin moments from experiment and theory. The angle dependence of the calculated effective moments is in good agreement with the experimental findings. An intermediate spin state is obtained independent from the presence of an oxygen layer on the surface, which affects the hybridization between surface and molecule. A high-spin state can be realized by adding Cl or O ligands, which cause a stretching of the metal center-N bond.

15 min. break

DS 19.6 Wed 11:00 H23

Magnetic coupling of Cobaltocene on magnetic surfaces through a graphene layer — •Simone Marocchi[1,2], Paolo Ferriani[3], Stefan Heinze[3], Franca Manghi[1,2], and Valerio Bellini[2,4] — [1]University of Modena and Reggio Emilia, Modena, Italy — [2]CNR Istituto di Nanoscienze S3, Modena, Italy — [3]Institute of Theoretical Physics and Astrophysics, Kiel, Germany — [4]CNR Istituto di Struttura della Materia, Trieste, Italy

The ability to improve the current electronic devices appear to be increasingly connected with the development of the molecule-based electronics [1] and spintronics [2]. We have concentrated our study, employing state-of-the-art density functional theory calculations, on the structural and magnetic properties of the Cobaltocene ($CoCp_2$) adsorbed on graphene deposited on slab of Ni(111). This molecule has been chosen because of its electronic structure rather unique among the metallocenes [3]. In several article has been pointed also out that graphene on Nickel (111) has mainly two energetically favored adsorption modes, namely top-fcc and bridge-top [4]. We will show how the magnitude of the magnetic coupling is drastically influenced by the structural factors named above and may vary by tens of meV. We further show how this coupling could be tuned by the intercalation of a magnetic monolayer, e.g. Fe and Co, between graphene and the Ni subtrate, and discuss the role of the graphene layer.

[1] X. Y. Zhu, Surf. Sci. Rep. 56, 1 (2004). [2] S. Sanvito, Chem. Soc. Rev. 40, 3336 (2011). [3] Y. Li, et al., Phys. Rev. B 83, 195443 (2011). [4] W. Zhao, et al., J. Phys. Chem. Lett. 2, 759 (2011).

DS 19.7 Wed 11:15 H23

Atomic-scale Inversion of Spin Polarisation above an Organic-Antiferromagnetic Interface — •Nuala Mai Caffrey, Paolo Ferriani, and Stefan Heinze — Institute of Theoretical Physics and Astrophysics, Christian-Albrechts-Universität zu Kiel

The emerging field of organic spintronics aims to combine the advantages of molecular electronics such as device miniaturisation and fabrication ease with the massive potential for application inherent in spintronics. Potential devices use organic molecules to control and manipulate spin-polarised signals. Such molecules are generally contacted with non-organic materials. As such, it is vital to understand the magneto-organic interface. It has been previously found that even the simplest non-magnetic molecule is capable of inverting the spin polarisation emerging from the clean ferromagnetic surface. We consider here an antiferromagnetic surface: a monolayer of Mn on a W(110) substrate. We perform *ab-initio* calculations in order to investigate the interface between simple organic molecules, both magnetic and non-magnetic, and an antiferromagnetic surface. The molecules considered include benzene (C_6H_6), cyclooctatetraene (C_8H_8) and small transition metal - benzene complexes. Simulated spin-polarised scanning tunnelling micoscopy (SP-STM) images are presented. They show that the exact magnitude and sign of the spin polarisation in the vacuum above the molecule is strongly dependent on the bonding details at the interface and due to the antiferromagnetic surface it exhibits a strong intra-molecular spatial dependence.

DS 19.8 Wed 11:30 H23

Spin Crossover in a Vacuum-Deposited Submonolayer of a Molecular Iron(II) Complex — •Matthias Bernien[1], Dennis Wiedemann[2], Christian F. Hermanns[1], Alex Krüger[1], Daniela Rolf[1], Wolfgang Kroener[3], Paul Müller[3], Andreas Grohmann[2], and Wolfgang Kuch[1] — [1]Institut für Experimentalphysik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany — [2]Institut für Chemie, Technische Universität Berlin, Straße des 17. Juni 135, 10623 Berlin, Germany — [3]Department of Physics, Universität Erlangen-Nürnberg, Erwin-Rommel-Straße 1, 91058 Erlangen, Germany

Spin-state switching of transition-metal complexes (spin crossover) is sensitive to a variety of tiny perturbations. It is often found to be suppressed for molecules directly adsorbed on solid surfaces. We present X-ray absorption spectroscopy measurements of a submonolayer of $[Fe^{II}(NCS)_2L]$ (L: 1-{6-[1,1-di(pyridin-2-yl)ethyl]-pyridin-2-yl}-*N*,*N*-dimethylmethanamine) deposited on a highly oriented pyrolytic graphite substrate in ultrahigh vacuum. These molecules undergo a thermally induced, fully reversible, gradual spin crossover with a transition temperature of $T_{1/2} = 235(6)$ K and a transition width of $\Delta T_{80} = 115(8)$ K. Our results show that, by using a carbon-based substrate, the spin-crossover behavior can be preserved even for molecules that are in direct contact with a solid surface.

Financial support by the DFG (Sfb 658: Elementary Processes in Molecular Switches on Surfaces) is gratefully acknowledged.

DS 19.9 Wed 11:45 H23

Single spin-crossover molecules triggered with a STM — •Manuel Gruber[1,2], Toshio Miyamachi[1], Martin Bowen[2], Samy Boukari[2], Eric Beaurepaire[2], and Wulf Wulfhekel[1] — [1]Physikalisches Institut, Karlsruher Institut für Technologie, Germany — [2]IPCMS (UMR 7504 UdS-CNRS) and Labex NIE, Strasbourg, France

A nano-scale molecular switch can be used to store information in a single molecule. The conductance of the molecule changes when switched and can be electrically detected. Spin crossover (SCO) molecules consisting of organic ligands around a transition metal ion are known to be switchable between a high- and a low-spin state by external stimuli [1]. It is the ultimate aim to achieve combined spin and conduction switching functionality on the level of individual molecules.

Fe(1,10-phenanthroline)2(NCS)2 molecules, SCO complexes, were deposited on Cu(100) and CuN/Cu(100) surfaces and studied with a scanning tunneling microscope (STM) in ultra-high vacuum at 4K.

Both spin species coexist at low temperatures as deduced from spectroscopic STM data. While on bare Cu(100), the molecules cannot be switched between the two spin states, molecules on CuN can individually and reproducibly be switched between a high-spin, high-conduction state and a low-spin, low-conduction state. This difference is explained by the role of the CuN layer to decouple the molecules from the metallic surface [2].

[1] P. Gütlich et al., Chem. Soc. Rev. 29, 419 (2000). [2] T. Miyamachi et al., Nat. Commun. 3, 938 (2012).

DS 19.10 Wed 12:00 H23

Beyond the Heisenberg model: Anisotropic exchange interaction between a Cu-tetraazaporphyrin monolayer and Fe3O4(100) — •Hans-Joachim Elmers[1], Julia Klanke[2], Eva Rentschler[2], Katerina Medjanik[1], Dmytro Kutnyakhov[1], Gerd Schönhense[1], Sergey A. Krasnikov[3], Igor V. Shvets[3], Stefan Schuppler[4], Peter Nagel[4], and Michael Merz[4] — [1]Institut für Physik, Johannes Gutenberg-Universität Mainz, D-55128 Mainz, Germany — [2]Institut für Anorganische Chemie und Analytische Chemie, Johannes Gutenberg-Universität Mainz, D-55099 Mainz, Germany — [3]Centre for Research on Adaptive Nanostructures and Nanodevices (CRANN) — [4]Karlsruhe Institute of Technology, Institut für Festkörperphysik (IFP), D-76021 Karlsruhe, Germany

We investigated the Heisenberg exchange coupling between the single Cu spin of Cu-tetraazaporphyrin deposited on magnetite(100) and the ferromagnetic surface using x-ray magnetic circular dichroism (XMCD). In contrast to the common model we find an anisotropic exchange coupling depending on the orientation of the spin relative to the bonding direction. The exchange coupling is ferromagnetic for magnetization direction perpendicular to the surface and antiferromagnetic for in-plane magnetization direction. The anisotropy of the Heisenberg exchange coupling is attributed to an orbitally-dependent exchange Hamiltonian. We propose that the sign change results from the competition between ferromagnetic superexchange along Fe-N-Cu and antiferromagnetic superexchange along Fe-O-Cu with strength modified by the strong spin-orbit coupling. Funded by COMATT.

DS 20: High- and Low-k-Dielektrics (jointly with DF)

Time: Wednesday 9:30–10:30 Location: H11

DS 20.1 Wed 9:30 H11

Dielectric signature of charge order in lanthanum nickelates — •Pit Sippel, Stephan Krohns, Peter Lunkenheimer, and Alois Loidl — Experimental Physics V, University of Augsburg, Germany

The technical progress of electronics requires new materials which have enhanced electrical properties, are cheaper, and are composed of nonscarce elements. In the last years charge-ordered nickelates, due to their extraordinary high-dielectric constant, have been found to be promising materials for the use as dielectrics in capacitive circuit elements [1]. However, the mechanism giving rise to their high dielectric constants is still under debate. Therefore we have performed a thorough structural, magnetic, and dielectric investigation of various isostructural $La_{2-x}(Ba,Ca,Sr)_xNiO_4$ compounds. For commensurably charge-ordered nickelates, a correlation between electronic phase separation and the permittivity is observed [2]. The dielectric spectra of these compounds show a superposition of two relaxational processes. The stronger one is most probably related to a non-intrinsic effect. The second one seems to originate from an intrinsic process. To gain further insight into the origin of the mechanisms leading to the observed relaxation spectra, ceramics and singlecrystalline samples have been examined.

[1] S. Krohns et al., Nat. Mat. **10**, 899 (2011).

[2] P. Sippel et al., Eur. Phys. J. B **85**, 235 (2012).

DS 20.2 Wed 9:50 H11

Mixed Sr/Ba oxides as high-k dielectric material on Si(100) — •Shariful Islam[1], Karl Hofmann[2], and Herbert Pfnür[1] — [1]Institut für Festkörperphysik, Leibniz Universität Hannover — [2]Inst. f. Bauelemente der Mikroelektronik, Leibniz Universität Hannover

Mixed Sr/Ba oxide layers can be grown perfectly lattice matched as crystalline and epitaxial layers on Si(100). At a mixing Sr/Ba ratio of 30:70, a band gap of 4.3eV was found. Here we demonstrate that band alignment is possible both for p- and n-type Si with a band offset of > 1eV. Dielectric constants of 27 ± 1 were determined for layer thickness between 4 and 16 nm, corresponding to capacitance equivalent thickness (CET) between 0.5 and 2.6 nm. The capacitance-voltage curves in MOS diodes fabricated by covering the oxide layers with 100 nm of Au show small hysteresis (< 1 mV) indicating a small density of rechargeable traps in the oxide films. Trap densities at the Si/oxide interface were determined by the conductance method to be close to 4×10^{10} $eV^{-1}cm^{-2}$. These properties are coupled with low leakage currents (< 4 mA/cm^2 at 5 nm thickness). These electrically excellent properties contrast with its limited thermal stability. At temperatures above 450°C the oxides are transformed into a well defined and again crystalline $(Ba_{0.8}Sr_{0.2})_2SiO_4$, which turns out to be stable up to desorption above 750°C, forming a band gap of 6 eV. First electrical measurements on this material will be discussed, too.

DS 20.3 Wed 10:10 H11

Combinatorial Preparation of Dielectric Films — •Achim Walter Hassel and Andrei Ionut Mardare — Institute for Chemical Technologygy of Inorganic Materials, Johannes Kepler University Linz, Austria

Valve metals such as Al, Hf, Nb, Ta, Ti, Zr are well known sources for thin anodic oxide films that can be used as dielectrics. Al and Ta are used in capacitors, Hf is handled as the new gold standard for high-k dielectrics. Each of the oxides on the pure metals has its advantages and disadvantages. In an attempt to optimise these properties an new approach is presented. Binary and ternary thin film libraries of these metals are prepared as compositional spreads on glass or silicon. Using scanning characterisation techniques such XRF, XRD, EXD the parent metal properties are linked to the oxide formation data, its specific resistance and dielectric constant. All these information is extracted from a series of experiments performed using scanning droplet cell microscopy (SDCM). A comprehensive data set is generated for each of these libraries, showing how properties are depending on the composition.

DS 21: Focus Session: Functionalized Semiconductor Nanowires II (jointly with HL)

Time: Wednesday 11:45–12:45 Location: H8

DS 21.1 Wed 11:45 H8

First-principles calculations of electronic and optical properties of ZnO nanowires — •Michael Lorke, Andreia Luisa da Rosa, and Thomas Frauenheim — Bremen Center for Computational Materials Science, University of Bremen, Germany

Semiconductor nanowires are promising candidates for the next generation of optoelectronic devices. In this work we have investigated the electronic and optical properties of bare and passivated ZnO nanowires with small diameter. We show that density-functional theory using the PBE0 functional can reproduce well the experimental ZnO band gap. Furthermore, by using the GW method in combination with the Bethe-Salpeter equation, we show that excitonic effects are strongly dependent on the nanowire size and surface termination.

DS 21.2 Wed 12:00 H8

BEC relaxation in a multimodal whispering-gallery exciton-polariton system — •Christof P. Dietrich, Tom Michalsky, Chris Sturm, Helena Franke, Martin Lange, Rüdiger Schmidt-Grund, and Marius Grundmann — Universität Leipzig, Inst. für Experimentelle Physik II, Linnéstr. 5, 04103 Leipzig

We present one-dimensional Bose-Einstein condensates (BEC) of whispering gallery mode (WGM) exciton-polaritons in ZnO-microwires up to room temperature. We show massive occupation of the bosonic ground state at condensation threshold, its blueshift and the condensate's one-dimensional extension and spatial coherence. We find that the condensation mechanism is different from that observed in common (two-dimensional) Fabry-Perot microcavities since the WGM system provides numerous photonic modes. Its ground state is energetically far below the exciton transition, so the system is multimodal without polariton ground state. This leads to two effects: 1.) At room temperature, the scattering of reservoir polaritons into zero-momentum states is strongly assisted by LO-phonons and very efficient because the energy-momentum conservation can be very easily fulfilled. 2.) At low temperature, a parametric relaxation process of polaritons into lower polariton branches is observed when an occupation of one is reached. States with a fixed energy difference ΔE_R are occupied. As the polariton-branch separation ΔE_P increases for lower mode numbers, the condensate gains kinetic energy when $\Delta E_P > \Delta E_R$. The lowermost state which can be reached is determined by the coupling strength and the lifetimes of exciton and WGM photon.

DS 21.3 Wed 12:15 H8

Oxygen-controlled electron-transfer dynamics under optical exitation in hybrid ZnO nano-/CdSe quantum dot structures — •Stephanie Bley[1], Dongchao Hou[1], Michael Diez[1], Sebastian Resch[2], Siegfried Waldvogel[2], Jürgen Gutowski[1], and Tobias Voss[1] — [1]Institute of Solid State Physics, Semiconductor Optics, University of Bremen, 28359 Bremen, Germany — [2]Institute of Organic Chemistry, Johannes Gutenberg University Mainz, 55128 Mainz, Germany

Due to their optoelectronic properties hybrid ZnO nano-/CdSe quantum dot structures possess a high potential for applications in photovoltaics and sensing. For this, the use of organic linker molecules to selectively attach the quantum dots to specific surfaces is a very versatile technique. We chemically synthesize colloidal CdSe quantum dots and attach them to the surface of ZnO nanostructures via different ω-mercapto alkanoic acids. The electron transfer dynamics of this hybrid systems are studied under illumination with a photon energy below the bandgap of ZnO (argon ion laser: λ=458 nm, E=2.7 eV). A strong enhancement of the photoconductivity has been found, and the experimental results demonstrate efficient electron tunneling from excited states of the quantum dots into the conduction band of the nanostructures. We discuss the influence of the length and electronic structure of the linker molecules on the electron transfer dynamics in the hybrid structures. Furthermore, we analyse the passivation of the ZnO nanostructure surfaces to reduce the influence of oxygen desorption for further studies of luminescence decay dynamics.

DS 21.4 Wed 12:30 H8

Polarization dependent CdS nanowire lasing — •Robert Röder[1], Sebastian Geburt[1], Robert Buschlinger[2], Ulf Peschel[2], and Carsten Ronning[1] — [1]Institut für Festkörperphysik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena — [2]Institut für Optik, Information und Photonik, Friedrich-Alexander-Universität Erlangen-Nürnberg, Haberstraße 9a, 91058 Erlangen

The forthcoming limitations of electronic integrated circuits cause reinforced work in nanophotonics for the development of on-chip optical components. Since semiconductor nanowires offer efficient waveguiding and mark the physical size limit of a photonic laser, they are promising candidates to overcome these limitations via optical data transmission and processing. High quality CdS NWs synthesized via VLS mechanism open up the green spectral range around 2.4 eV acting as Fabry-Pérot laser resonators with a remarkable low threshold of 10 kW/cm^2 at room temperature. Since optical processing is specified by the direct emission of the device, a "head-on" setup was developed for the investigation of the light output originating out of the facet end along the nanowire axis. The slope efficiency of the optically pumped CdS nanolaser was determined with a high value of 5-10 %. The lasing emission as well as the ASE is furthermore highly dependent on the polarization of the optical pumping with polarization ratios around 0.15 for the emission. FDTD simulations reveal, that the increased pumping efficiency for along the nanowire axis polarized excitation is more likely based on the absorption profile than on the absolute absorption.

DS 22: Gaede Prize Talk - Kirsten von Bergmann

Time: Wednesday 13:15–13:55 Location: H15

Prize Talk DS 22.1 Wed 13:15 H15

Complex magnetic order on the atomic scale — •Kirsten von Bergmann — Institute of Applied Physics, University of Hamburg

Magnetism in low-dimensions is a versatile topic and broken inversion symmetry due to the presence of a surface can induce the formation of complex magnetic order. Here the driving force for the canting of adjacent magnetic moments is the spin-orbit induced Dzyaloshinskii-Moriya interaction. Thin magnetic films on heavy substrates are good candidates for this kind of surface-induced non-collinear magnetic states with unique rotational sense.

Spin-polarized scanning tunneling microscopy (SP-STM) combines magnetic sensitivity with high lateral resolution and therefore grants access to such complex magnetic order with unit cells on the nanometer scale. Several non-collinear magnetic ground states, such as spin spirals where the spin rotates from one atom to the next, habe been observed [1-3]; while in uniaxial systems only one propagation direction is found, in biaxial systems rotational domains of spin spirals are present. In the case of the monolayer Fe on Ir(111) a combination of different magnetic interactions, including higher-order interactions, leads to a two-dimensional lattice of magnetic skyrmions on the atomic scale [4,5].

[1] M. Bode et al., Nature 447, 190 (2007).
[2] P. Ferriani et al., Phys. Rev. Lett. 101, 27201 (2008).
[3] M. Menzel et al., Phys. Rev. Lett. 108, 197204 (2012).
[4] K. von Bergmann et al., Phys. Rev. Lett. 96, 167203 (2006).
[5] S. Heinze et al., Nature Phys. 7, 713 (2011).

DS 23: Focus Session: Thin Film Photovoltaic Materials and Solar Cells II

Time: Wednesday 14:45–18:15 Location: H8

DS 23.1 Wed 14:45 H8

Oxygen vacancy doping of TiO$_2$ — •Simon Moser[1,2], Luca Moreschini[2], Jacim Jacimovic[1], Osor Barisic[3], Helmuth Berger[1], Arnaud Magrez[1], Young Jun Chang[2,4], Keun Su Kim[2], Aaron Bostwick[2], Eli Rotenberg[2], Laszlo Forro[1], and Marco Grioni[1] — [1]Ecole Polytechnique Federale de Lausanne — [2]Advanced Light Source, Lawrence Berkeley National Laboratory — [3]University of Zagreb — [4]University of Seoul

The titanium oxide TiO$_2$ has been object of extensive studies because of its suitability in many practical fields, ranging from photovoltaic applications, to catalysis, memristors, and others. As for many other transition metal oxides, great attention has been devoted to the impact on the electronic structure of different doping mechanisms, either extrinsic or due to the creation of oxygen vacancies. Here we report an angle-resolved photoemission (ARPES) work on TiO$_2$ single crystals and epitaxial films grown with the *in situ* pulsed-laser-deposition (PLD) system available at beamline 7.0.1 of the Advanced Light Source. We show the evolution of the electronic structure as a function of the amount of oxygen vacancies induced by the photon beam.

DS 23.2 Wed 15:00 H8

Work function determination of degenerately Al-doped ZnO by thermionic emission — •Christian Wilde, Bernd Schmidt, Mykola Vinnichenko, and Sibylle Gemming — Helmholtz-Zentrum Dresden-Rossendorf, Institute of Ion Beam Physics and Materials Research, Dresden, Germany

Degenerately Al-doped ZnO (AZO) is a transparent conductive oxide (TCO) widely used, especially as electrode material in solar cells. The work function of these electrodes is of crucial importance, because it determines the electronic barrier between the TCO and the semiconducting absorber. Therefore, this barrier directly affects the charge collection and thus solar cells efficiency. In this contribution we report the results of experiments carried out to determine the work function of AZO by using the thermionic emission theory. AZO, as a degenerately doped semiconductor with the Fermi level in the conduction band shows a metal-like behaviour, and, if it is brought into contact with a semiconductor, it forms a Schottky barrier. From measurements of temperature-dependent current-voltage characteristics the work function of AZO can be determined. We demonstrate that this model of metal/semiconductor contact is applicable to the contact between AZO and a non-degenerately doped substrate (silicon or germanium). The Schottky barrier formation is studied with respect to the substrate conductivity type and surface cleaning. The determined AZO work function variation will be discussed in relation to the film properties and process parameters of reactive and non-reactive DC magnetron sputter deposition.

DS 23.3 Wed 15:15 H8

Laser Based Shunt Removal of Silicon and Chalcopyrite based Thin Film Solar Cells — •Christof Schultz[1], Manuel Schüle[1], Sven Kühnapfel[3], Kamil Stelmaszczyk[1], Moshe Weizman[1], Holger Rhein[2], Björn Rau[2], Rutger Schlatmann[1,2], Volker Quaschning[1], Bert Stegemann[1], and Frank Fink[1] — [1]HTW Berlin - University of Applied Sciences, Wilhelminenhofstr. 75a, 12459 Berlin, Germany — [2]PVcomB/ Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Schwarzschildstr. 3, D* 12489 Berlin, Germany — [3]Helmholtz-Zentrum für Materialien und Energie, Institut für Silizium-Photovoltaik, D-12489 Berlin, Germany

In commercial thin film solar cell production defective areas can occur due to material impurities or by "rough" sample handling between the different deposition steps. Such defects can cause disproportionate losses or even shortcuts in the solar cells. The removal of these defects would increase the solar cell performance as well as the overall manufacturing yield. In our study we present a technique for identification of shunted regions by means of lock-in thermography and successful laser based removal of shunts in silicon and chalcopyrite thin film solar cells. These results show that the removal of point-like defects increases the overall device performance significantly.

DS 23.4 Wed 15:30 H8

First-principles electronic structure of β-FeSi$_2$ and FeS$_2$ surfaces — •Pengxiang Xu, Timo Schena, Stefan Blügel, and Gustav Bihlmayer — Peter Grünberg Institut & Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

Applying density functional theory in the framework of the full-potential linearized augmented plane-wave (FLAPW) method `FLEUR` [1], we investigate the electronic structure of potential future photovoltaic materials, β-FeSi$_2$ and FeS$_2$, for selected surface orientations and terminations with and without surface passivation. We also study the electronic structure of bulk β-FeSi$_2$ including recently observed stacking faults.

By comparing surface energies, the most stable orientations are determined for different terminations among different orientations. Detailed electronic structure calculations show that surface states originating from Fe play an important role and might determine the photovoltaic properties. For selected systems, we present the effects of passivation on the electronic structure and study how the bandgap is affected by stacking faults found in β-FeSi$_2$. Our results furthermore indicate that anti-ferrimagnetic ordering exists for Fe-terminated surfaces.

This work is supported by BMBF under project Nr. 03SF0402A (NADNuM).

[1] www.flapw.de

DS 23.5 Wed 15:45 H8

Oxide Heterostructures for Efficient Solar Cells — •Elias Assmann[1], Peter Blaha[2], Karsten Held[1], Satoshi Okamoto[3], and Giorgio Sangiovanni[4] — [1]Institut für Festkörperphysik, Technische Universität Wien — [2]Institut für Materialchemie, Technische Universität Wien — [3]Materials Science and Technology Division, Oak Ridge National Laboratory, USA — [4]Institut für Theoretische und Astrophysik, Universität Würzburg

We propose an unexplored class of absorbing materials for high-efficiency solar cells: heterostructures of transition-metal oxides. In particular, LaVO$_3$ grown on SrTiO$_3$ has a direct band gap $\sim$ 1.1 eV in the optimal range as well as an internal potential gradient, which can greatly help to separate the photo-generated electron-hole pairs. Furthermore, oxide heterostructures afford the flexibility to combine LaVO$_3$ with other materials such as LaFeO$_3$ in order to achieve even higher efficiencies with band-gap graded solar cells. We use density-functional theory to demonstrate these features.

DS 23.6 Wed 16:00 H8

New insights into the mechanisms of photodegradation / stabilization of P3HT:PCBM active layers using poly(3-hexyl-d13-thiophene) — •Aurélien Tournebize[1], Pierre-Olivier Bussière[1], Pascal Wong-Wah-Chung[1], Agnès Rivaton[1], Jean-Luc Gardette[1], Kion Norrman[2], Frederik C. Krebs[2], Hussein Medlej[3], Roger C. Hiorns[3], and Christine Dagron-Lartigau[3] — [1]Institut de Chimie de Clermont-Ferrand, Equipe Photochimie Clermont-Ferrand, France — [2]IPREM, Université de Pau et des Pays de l'Adour, France — [3]Technical University of Denmark, Department of Energy, Denmark

The use of deuterated P3HT permitted distinction of carbon originating from the hexyl-d13 chain and carbon originating from PCBM and the non-deuterated thiophene unit. The photooxidation of both components of the blend was monitored using the combination of various analytical techniques (Tof-SIMS, XPS, infrared and UV-visible spectroscopy, gas phase analysis) to probe the bulk and the surface of the deposit.

The results show that the stabilization of P3HT by PCBM is due to morphological changes during photooxidation. In parallel, the wavelength effect has been investigated.

The results obtained in this work advance the understanding of active layer stability and will help improve the design of organic solar cells resulting in longer lifetimes thanks to the use of cut-off filter in the substrate or encapsulation of the devices.

DS 23.7 Wed 16:15 H8

Electrodeposition of aromatic compounds on silicon and subsequent cross linking - first steps towards a novel bottom-up synthesis of graphene — •Janek Zeuschner, Gerald V. Troppenz, Jörg Rappich, and Norbert H. Nickel — Helmholtz-Zentrum Berlin, Institut für Siliziumphotovoltaik, Kekuléstr. 5, 12489 Berlin, Germany

The state-of-the-art method for the production of high-quality macroscopic graphene sheets is CVD synthesis on copper. However, during the growth process holes and grain boundaries are introduced in the material, resulting in adverse effects on its electronic properties. Furthermore, future technological applications of graphene require a transfer step from copper to silicon. This is expected to disturb the ordered structure of the graphene sheets even further. Therefore it would be highly desirable to grow single-layer graphene on silicon directly. We present first steps of a novel approach to synthesize graphene from small molecules on single-crystal silicon. During electrodeposition of suitable aromatic organic compounds, the defect density on the silicon-solution interface is monitored by in-situ photoluminescence spectroscopy. The mechanism of deposition is analyzed and results from cross-linking experiments are shown.

Coffee break (15 min)

DS 23.8 Wed 16:45 H8

Diffusion of copper in In$_2$S$_3$ layers prepared by ion layer gas reaction method — •Albert Juma, Rodrigo Sáez-Araoz, Christian-Herbert Fischer, and Thomas Dittrich — Helmholtz-Centre-Berlin for Materials and Energy, Hahn-Meitner-Platz 1, 14109 Berlin, Germany.

Diffusion of copper in semiconductors remains an important phenomenon in photovoltaics because it affects the electronic properties, formation of interfaces, solar cell characteristics and stability. In$_2$S$_3$ layers were prepared by ILGAR (ion layer gas reaction) method with InCl$_3$ and In In(OCCH$_3$CHOCCH$_3$)$_3$ as precursor salts to obtain Cl-containing and Cl-free layers, respectively. Diffusion experiments were performed by annealing Si/In$_2$S$_3$/CuSCN layer systems at different temperatures and times and then etching away CuSCN in pyridine solution. The concentration profiles of Cu in In$_2$S$_3$ were obtained using Rutherford backscattering spectrometry (RBS) from which the diffusion coefficients were determined as a function of temperature. The diffusion in Cl-containing layers was limited by a lower solubility limit while the Cl-free layers showed one diffusion process with a relatively higher solubility. The activation energies for Cu diffusion were 0.041eV and 0.24 eV for In$_2$S$_3$ layers with and without Cl respectively. The influence of In-Cl bond on the local structure of In$_2$S$_3$:Cl and on the diffusion process of Cu$^+$ are discussed.

DS 23.9 Wed 17:00 H8

Time-Resolved Photoluminescence Studies on Cu(In,Ga)Se2 Thin Film Solar Cells — •Viktor Gerliz, Dimitrios Anastassiou, Jörg Ohland, Dirk Otteken, Ingo Riedel, and Jürgen Parisi — Carl von Ossietzky Universität Oldenburg

The aim of this study is to evaluate the qualification of time-resolved photoluminescence (TR-PL) measurements as tool for quality management for inline production of Cu(In,Ga)Se2 thin film modules. Prior to the interpretation of TR-PL measurements regarding device-characteristic quality parameters, the first stage of the study addresses the technical requirements for reliable data acquisition via time-correlated single photon counting. We observed that decay curves taken at low-injection (LI) levels generally exhibit mono-exponential decay characteristics, while high injection (HI) causes superposition with a slower relaxation process. Short measurement times are required for industry applications of this technique. These can only be achieved at sufficiently high excitation intensity (HI). Under such conditions we observe a correspondence between open circuit voltage and the second order decay constant.

DS 23.10 Wed 17:15 H8

Device analysis of CIGSe superstrate solar cells — •Marc D. Heinemann, Christian A. Kaufmann, Britta Höpfner, Thomas Unold, and Hans-Werner Schock — Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany

Cu(In,Ga)Se2 solar cells in the superstrate configuration offers a number of advantages regarding industrial device fabrication as well as the option of direct application in tandem device structures. The drawback is the lower efficiency due to the difficulty to design the heterointerface, which traditionally relies on buffer layers like CdS that are unstable at the high process temperatures. In this work superstrate Cu(In,Ga)Se2 solar cells are prepared by coevaporation at different temperatures directly on a variety of ZnO coated glass substrates. Depending on the process conditions, the formation of a thin GaO compound or InO compound layer has been observed at the interface. It was found that the InO layer enables the Zn diffusion into the absorber and induces a low shunt resistance, whereas the GaO layer acts as a diffusion barrier for Zn. Currently a max conversion efficiency of around 7% has been achieved. The device performance of these superstrate devices is modeled by numerical simulation, taking into account results from admittance and photoelectron spectroscopy of the interface. To overcome the efficiency limiting effects derived from this device model, different interface conditionings in combination with the application of a variety of buffer layers are carried out and will be presented.

DS 23.11 Wed 17:30 H8

Laser Patterning of CIGS absorber layers with short nanosecond laser pulses — •Manuel Schüle[1], Christof Schultz[1], Kamil Stelmaszczyk[1], Moshe Weizman[1], Holger Rhein[2], Björn Rau[2], Rutger Schlatmann[1,2], Volker Quaschning[1], Bert Stegemann[1], and Frank Fink[1] — [1]HTW Berlin - University of Applied Sciences, Wilhelminenhofstr. 75a, 12459 Berlin, Germany — [2]PVcomB / Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Schwarzschildstr. 3, D-12489 Berlin, Germany

Laser based patterning of chalcopyrite thin film solar cells is an essential step towards high efficiencies since the dead area of the solar module is reduced. When manufacturing solar modules, the second laser patterning step typically comprises the removal of very fine lines in the absorber material by ultra-short laser pulses in order to create a direct contact between the back contact of one cell and the front contact of the adjacent cell. Such ultra-short ps or fs laser pulses are necessary to avoid melting of the absorber which might create a binary conductive phase and thereby shunts in the solar cell. In our study we demonstrate successful laser patterning by using a low-cost nanosecond laser source (532 nm) for local phase transformation of the absorber material instead of removing the material. This patterning step is performed after complete deposition of all layers through the front contact allowing for a simplified and accelerated manufacturing process.

DS 23.12 Wed 17:45 H8

Stöchiometrieabhängigkeit des Ladungsträgertransports in CZTS-Solarzellen — •Justus Just[1,2], Melanie Nichterwitz[1], Steffen Kretzschmar[1], Dirk Lützenkirchen-Hecht[2], Ronald Frahm[2] und Thomas Unold[1] — [1]Helmholtz-Zentrum-Berlin für Materialien und Energie GmbH, Hahn-Meitner-Platz 1, D-14109 Berlin — [2]Fachbereich C - Physik, Bergische Universität Wuppertal, Gaußstraße 20, D-42097 Wuppertal, Germany

Mit Cu$_2$ZnSnS$_4$ (CZTS) in Chalkopyrit-verwandter Kesteritstruktur als Absorbermaterial in Dünnschichtsolarzellen werden bereits Wirkungsgrade von über 8,4 % erreicht, während der Zusammenhang zwischen Abweichungen von der Stöchiometrie des Materials und den resultierenden elektronischen Eigenschaften bislang kaum verstanden ist. Hier werden CZTS-Solarzellen unterschiedlicher Zusammensetzung mittels EBIC-Aufnahmen (ortsaufgelöste Elektronenstrahl-Angeregte Ladungsträgergeneration) am Querschnitt der Solarzelle untersucht. Daraus können die Diffusionslänge sowie die Ladungsträgerdichte abgeschätzt werden. Zusammen mit Messung der Kapazität bei Raumtemperatur, der externen Quanteneffizienz und der I-V-Kennlinie entsteht so ein konsistentes Modell der Ladungsträgertransporteigenschaften. Um diese in Zusammenhang mit der tatsächlichen Zusammensetzung der CZTS-Phase zu bringen, die sich aufgrund von Fremdphasen signifikant von der Probenzusammensetzung unterscheiden kann, wird eine vollständige Phasenanalyse mittels Röntgenabsorptionsspektroskopie durchgeführt.

DS 23.13 Wed 18:00 H8

Photoluminescence and Raman scattering in wurtzite Cu2ZnSn(S1-x,Sex)4 nanocrystals — •Sergej Levcenko[1], Thomas Unold[1], Ajay Singh[2,3], Shalini Singh[2,3], and Kevin M Ryan[2,3] — [1]Helmholtz Zentrum Berlin für Materialien und Energie, Berlin, Germany — [2]SFI-Strategic Research Cluster in Solar Energy Conversion, University of Limerick, Ireland — [3]Materials and Surface Science Institute, University of Limerick, Ireland

Cu2ZnSn(S1-x,Sex)4 (CZTSSe) semiconductors gain much attention due to their potential photovoltaic application. Recently, by nanocrystal chemistry approach the formation of the new wurtzite crystal phase of CZTS and CZTSe which is thermodynamically unstable in a bulk phase (kesterite/stannite) were reported. Here we present the vibrational and optical properties of wurtzite- CZTSSE nanocrystals as a function of x characterized by Raman and photoluminescence. The pseudo-spherical CZTSSE nanocrystals with the diameter of about 20 nm were prepared by colloidal chemistry method. The Raman spectra of the CZTSSE nanostructures show a two mode behavior. The intensive CZTSE-like mode strongly shifts from 191 cm-1 for x=1 to 225 cm-1 for x=0.15, while the intensive CZTS-like mode barely shifts from 333 cm-1 for x=0 to 329 cm-1 for x=0.8. The low temperature CZTSSE PL spectra show one broad PL band which is gradually tuned from 1.4 eV for x=0 to 0.9 for x=0.15. The observed PL band most likely originates from near band edge emission of wurtzite CZTSSE nanocrystals.

DS 24: Thermoelectric Materials

Time: Wednesday 14:45–17:00 Location: H32

DS 24.1 Wed 14:45 H32

Investigations on novel thermoelectric materials using a high temperature Hall-measurement-setup — •Hans-Fridtjof Pernau, Markus Bartel, Frank Menzel, Alexandre Jacquot, Martin Jägle, and Kilian Bartholome — Fraunhofer IPM

Novel thermoelectric materials especially for medium and high temperature application are in the focus for waste heat recovering systems not only in automotive applications. Beside the accurate determination of all thermoelectric properties and thereby the ZT-value a detailed understanding of the processes inside the materials are needed. Hall-measurements are the well-known tool to investigate carrier concentration and mobility within metals, semiconductors and of course thermoelectric materials. Up to now most commercial setups are only suitable for temperatures up to 400°C. The full characterization of high temperature materials like oxides or silicides require measurement temperatures of 600°C and above. Therefore Fraunhofer IPM developed a high temperature Hall-measurement-setup which allows measurements in this range. We will present first high temperature measurements on different materials and sample geometries performed with our new IPM-HT-Hall setup.

DS 24.2 Wed 15:00 H32

Thermoelectric properties of laser-assisted wet-chemically doped group-IV nanoparticles — •Benedikt Stoib[1], Anton Greppmair[1], Tim Langmann[1], Nils Petermann[2], Hartmut Wiggers[2], Martin Stutzmann[1], and Martin S. Brandt[1] — [1]Walter Schottky Institut, Technische Universität München, Am Coulombwall 4, 85748 Garching — [2]Institut für Verbrennung und Gasdynamik, Universität Duisburg-Essen, Lotharstraße 1, 47048 Duisburg

We present recent studies on the morphology and the thermoelectric properties of thin films of laser-sintered group-IV nanoparticles. The structure size in the macro-porous network is in the sub-μm regime and can be controlled by the laser fluence used for sintering. Doping was achieved by immersing the nanoparticle film prior to sintering in a liquid containing the dopants. Conductivity and thermopower measurements provide insight into the doping efficiency. For the doping with group-V elements we find a threshold concentration, above which the conductivity can be increased by several orders of magnitude up to 100 S/cm, using different dopant concentrations in the dopant solution. Thermopower measurements show that the laser-sintered thin films are indeed n-type after this procedure, reaching a maximum Seebeck coefficient of -270 μV/K. We present the extension of this doping method to SiGe and Si and discuss relevant materials properties affecting the efficiency of the doping process.

[1] B. Stoib et al., Phys. Stat. Solidi A, doi 10.1002/pssa.201228392 (2012)

DS 24.3 Wed 15:15 H32

Nanoscale Heat Transport from Self-Organised Ge Hut and Dome Clusters into Si(001)

— •Tim Frigge, Boris Krenzer, Verena Tinnemann, Annika Kalus, Friedrich Klasing, Anja Hanisch-Blicharski, and Michael Horn-von Hoegen — University of Duisburg-Essen and CENIDE, Duisburg, Germany

The nanoscale heat transport from self-organized Ge hut and dome clusters into Si substrates was determined by ultrafast time-resolved electron diffraction in reflection geometry. Within a temperature range between 400°C and 600°C Ge grows epitaxially in form of kinetically self-limited hut and dome clusters. In-situ deposition of 8ML Ge at 550°C under UHV conditions on Si(001) results in huts of 2 nm height and 20 nm width and domes with a height of 6 nm and a diameter of 50 nm. The clusters were excited in a pump-probe setup by 50 fs-laser pulses at a wavelength of 800 nm and probed by ultrashort electron pulses. Electron diffraction patterns were recorded at different delay times between the pump and probe pulses The observed transient drop of spot intensity is explained by the Debye-Waller effect and reflects the temperature increase from 25 K to 125 K. The cooling rate is determined from the exponential recovery of intensity: huts cool within 50 ps while the larger domes cool three times slower in 150 ps. This is in clear contrast to temperature dependent numerical simulations and reflects that size effects can reduce the heat transfer in nanoscale heterosystems by more than a factor of 8.

DS 24.4 Wed 15:30 H32

Thermal conductivity of SiGe-based nanostructures

— •Katrin Bertram[1], Bodo Fuhrmann[1], Nadine Geyer[2], Alexander Tonkikh[2], Nicole Wollschläger[2], Peter Werner[2], and Hartmut S. Leipner[1] — [1]Interdisziplinäres Zentrum für Materialwissenschaften, Martin-Luther-Universität Halle- Wittenberg, 06120 Halle, Germany — [2]Max Planck Institute of Microstructure Physics, Weinberg 2, 06120 Halle, Germany

A low thermal conductivity of thermoelectric materials is necessary to achieve enhanced figure of merits ZT for thermoelectric generators and Peltier coolers. Regarding theoretical predictions, nanostructured materials such as superlattices, quantumdot superlattices or nanowires, are able to show a higher figure of merit than bulk materials. The reduction of thermal conductivity in superlattices is achieved by diffuse interface scattering of the phonons at the interfaces. With a mismatch of the phonon dispersions the scattering of short-wavelength phonons is enhanced due to localized phonon states. Some theoretical work predicted a further decrease in thermal conductivity with nonperiodic superlattice structures. In this study, we have investigated the thermal conductivities of Si-Ge based superlattices. Periodic and nonperiodic Si_m-Ge_n superlattices with stacks of m Si and n Ge layers of various thicknesses were grown by molecular beam epitaxy on (111) Si substrates. The influence of periodicity was investigated. Further investigations were done on nanowire arrays grown from these superlattices. A comparison between the different approaches for the reduction of thermal conductivity will be presented.

DS 24.5 Wed 15:45 H32

Thermoelctrical Measurements on Single Bi_2Te_3 Nanowires

— •Danny Kojda[1], Rüdiger Mitdank[1], Zhi Wang[2], Michael Kröner[2], Peter Woias[2], William Töllner[3], Kornelius Nielsch[3], and Saskia F. Fischer[1] — [1]Novel Materials, Humboldt-Universität zu Berlin, D-10099 Berlin — [2]IMTEK, University of Freiburg, D-79110 Freiburg — [3]University of Hamburg, D-20355 Hamburg

Nanowires (NWs) made of Bi_2Te_3 are expected to improve the thermoelectric efficiency. In order to investigate the thermoelectric properties (Seebeck coefficient, electrical and thermal conductivity), as well as the crystal structure via TEM for one and the same NW, a special measurement device was fabricated by means of silicon micromachining [1]. This device contains two symmetric Si cantilevers (with a $4\,\mu$m gap) where the NW is deposited in between via dielectrophoresis and contacted in four point geometry via electron beam assisted deposition of Pt. Thin Pt micro-heaters and Pt-thermometers are situated near the NW to create and measure a temperature gradient. In the bath temperature range $T_B = 4.2\,$K-300 K we measured the temperature dependent resistance of a single Bi_2Te_3-NW, observing metallic behavior. We also measured the Seebeck voltage between the NW-endings and a resistance change of the heated thermometer lead as function of the heating current and bath temperature. With this we are able to calculate tempeature dependent the Seebeck coefficient. It has an absolute maximum of $-35\,\mu$V/K at about 200 K.

[1] Z. Wang *et al.*, Sens. and Actuat. A: Phys. (188; p. 417-426; 2012)

DS 24.6 Wed 16:00 H32

Reduced thermal conductivity in Half Heusler superlattices

— •Tino Jaeger[1], Christoph Euler[1], Christian Mix[1], Michael Schwall[2], Benjamin Balke[2], Sascha Populoh[3], Anke Weidenkaff[3], Claudia Felser[2], and Gerhard Jakob[1] — [1]Institut für Physik, Johannes Gutenberg Universität Mainz, Staudinger Weg 7, 55099 Mainz, Germany — [2]Institut für Anorganische Chemie und Analytische Chemie, Johannes Gutenberg Universität Mainz, Staudinger Weg 7, 55099 Mainz, Germany — [3]Empa-Eidgenössische Materialprüfung und -forschungs Anstalt Festkörperchemie und Katalyse, Ueberlandstrasse 129, 8600 Duebendorf, Switzerland

Besides bulk applications that are well-established in industry, thin film technology moves into focus. Self-sustaining sensors and on-chip cooling represent the most emerging fields of application. As valid for the conventional techniques, enhancing ZT would open new prospects in commercial usage. For thin films, the fabrication of superlattices enables a unique type of nanostructuring. To sustain electronic behavior from layer to layer, subsequently deposited materials must have a structural similarity. XRD and transport measurements have shown that the Half-Heusler alloys TiNiSn and $Zr_{0.5}Hf_{0.5}NiSn$ are appropriate in doing so. Increased cross-plane ZT in this material system is requested by additional interface scattering. Depressed thermal conductivity has been obtained by 3omega method. The measurement was performed by a home-made assembly using a passive circuit and a lock-in amplifier. We gratefully acknowledge financial support by DFG Ja821/4-1 with in the priority program SPP 1386.

DS 24.7 Wed 16:15 H32

Growth and characterization of the low-temperature properties of $MoSi_2$ thin films

— •Mehrdad Baghaie Yazdi, Maximilian Fries, and Lambert Alff — Technische Universität Darmstadt, Materialwissenschaft, Dünne Schichten, Darmstadt, Deutschland

$MoSi_2$ is considered to be one of the best high-temperature electric conductors, often used as heating element in furnaces. Its oxidation resistance at elevated temperature makes it a good candidate as a thin film electrode for various applications. However, $MoSi_2$ also shows intriguing low-temperature properties when grown as a thin film. Woerlee *et al.* [1] attributed a low-temperature anomaly to the Kondo effect. In a new set of experiments we have studied the growth properties of radio-frequency magnetron sputtered $MoSi_2$ on polycrystalline Al_2O_3. We have characterized the thin films by X-ray diffraction and scanning electron microscopy. Based on low-temperature electrical transport measurements we propose a novel nanocrystal network conduction model as alternative scenario.

[1] P. H. Woerlee *et al.*, Appl. Phys. Lett. **44, 876 (1984).**

DS 24.8 Wed 16:30 H32

Acoustic phonon propagation in cobalt antimony skutterudites

— •Chuan He[1], Martin Grossmann[1], Martin Schubert[1], Marcus Daniel[2], Manfred Albrecht[2], and Thomas Dekorsy[1] — [1]University of Konstanz, Germany — [2]Chemnitz University of Technology, Germany

Cobalt antimony skutterudites are interesting due to their promising thermoelectric properties. Filling foreign atoms in its cage-like structure is considered beneficial to their thermoelectric properties. The undoped CoSb3 samples and Co4Sb12 samples with different Yb concentration we studied are fabricated using molecular beam epitaxy and characterized by femtosecond pump and probe spectroscopy with an asynchronous optical sampling system. The transient reflectivity signal is strongly dependent on the Yb concentration. For highly doped samples fast electron-phonon coupling is observed.

DS 24.9 Wed 16:45 H32

The ineffectiveness of energy filtering at grain boundaries for thermoelectric materials

— •Michael Bachmann, Michael Czerner, and Christian Heilger — I. Physikalisches Institut, Justus Liebig University Giessen, D-35392, Germany

We present results that show the ineffectiveness of energy filtering at grain boundaries [1]. Our results are based on a model that we developed to describe electron transport in nanograined materials. For the band structure we use a one band effective mass model. The transport is calculated using the Landauer formalism. The grain boundaries are described using the model by Seto [2]. In this model additional trapping states in the grain boundary are assumed that causes a space charge accumulation in the grain boundary. This space charge distribution leads to a formation of a double Schottky barrier. It is believed that such barriers can increase the efficiency of thermoelectric materials by energy filtering effects. Since in our model the space charge distribution depends on the doping concentration and therefore also the barrier, we are able to calculate the electron transport in dependence of the doping concentration. For low doping concentration we obtain a energy filtering effect, but for high doping concentration that are necessary for effective thermoelectric material the barrier height and width is too small to have an impact on the transport. Therefore, we conclude that electrostatic barriers play no role for thermoelectric devices.

[1] M.Bachmann, M. Czener and C.Heiliger, Phys. Rev. B 86, 115320
[2] J. Seto, J.Appl. Phys. 46 5247 (1975)

DS 25: Focus Session: Magnetic Damping Phenomena in Thin Films and Nanostructures (jointly with MA)

Organizers: J. Lindner (HZDR), H. Ebert (TU München)

New emerging technologies for enhanced magnetic information storage require an improved understanding and control of the mechanisms that influence the magnetization reversal and stability on the nanoscale. The key property in this context is magnetic relaxation as it governs all processes that invoke the dynamic behavior of the magnetization. In this session we aim to discuss recent progress in understanding intrinsic Gilbert damping as well as extrinsic relaxation channels which are relevant for the timescales of femto- to nanoseconds. Besides experimental approaches in time and frequency domain, state-of-the art theoretical descriptions on an ab-initio basis as well as model calculations are reviewed.

Time: Wednesday 15:00–17:30 Location: H10

Topical Talk DS 25.1 Wed 15:00 H10

An overview of magnetic damping in ferromagnets — •Robert McMichael — National Institute of Standards and Technology, Center for Nanoscale Science and Technology, Gaithersburg MD USA

Many of the applications for magnetic nanotechnology depend on the ability to write and read information quickly by switching and measuring the magnetization in magnetic nanostructures, and the magnetic damping plays an important role in the dynamics. The desired amount of damping depends on the application. For example, in some cases, strong damping enables fast switching, while in other cases strong damping prevents switching. In this talk, I will give a brief introduction to the phenomenology of damping, or relaxation, of magnetization in ferromagnets, which is often nicely described by a viscous drag or Gilbert damping. I aim to supplement this phenomenological picture by reviewing the current understanding of damping mechanisms in ferromagnetic metals. The primary mechanism involves transferring energy to electronic states near the Fermi surface. Additionally, in nanostructures, the dynamic effects of damping can be modified by spin polarized currents either that are injected from external sources or that are generated spontaneously by the magnetization precession. I will conclude by focusing on problems of interpreting damping measurements in materials with defects, and on the opportunities for intrinsic damping measurements in nanostructures.

Topical Talk DS 25.2 Wed 15:30 H10

Magnetic Damping on Femtosecond Time Scales — •Markus Münzenberg — Georg-August University, I. Phys. Institute, Göttingen, Germany

Achieving high speed magnetization dynamics in magnetic materials is at the heart of the engineering of spin-based electronic devices. Microscopic processes in a magnetic materials involve electrons, their spins, and their interactions with phonons. Materials with low damping constants can be realized by controlling the spin-flip channels at the Fermi level. Metallic Heusler compounds show a Gilbert damping of 0.002-0.006, however, the theoretically predicted values are $10^{-5} - 10^{-4}$.

The experiments we report in this talk demonstrate a successful control of spin polarization and spin dynamics on ultrafast time scales in magnetic materials through their electronic structure. For achieving a systematic variation in their electronic structure as a control, we have made a selection of so-called half-metals, in the family of the Heusler compounds and pseudogap materials that are close relatives, but their electronic structure is robust against structural disorder. Interestingly, similar values of spin polarization are seen in the pseudogap materials as well, making them another promising class of high-spin-polarization materials.

[1] A. Mann, J. Walowski, M. Münzenberg, S. Maat, M. J. Carey, J. R. Childress, C. Mewes, D. Ebke, V. Drewello, G. Reiss, A. Thomas, Phys. Rev. X 2, 041008 (2012).

Topical Talk DS 25.3 Wed 16:00 H10

Two-Magnon Excitations: From Periodical Perturbations to Magnonic Crystals — •Kilian Lenz — Magnetism Division, Institute for Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, P.O. Box 510119, 01324 Dresden

Two-magnon scattering is a well-known effect e.g. in ferromagnetic resonance experiments leading to a linewidth broadening. Available theory so far was based on random defects acting as a dipolar scattering potential. Recently it was shown by Landeros and Mills [1] that this theory can be extended to handle two-magnon scattering in *periodically* perturbed films, which can be easily created by lithographical patterning. These perturbed films are the intermediate step towards full magnonic crystals. The extended model allows for analytically calculating the response function of 1D and 2D periodically perturbed ferromagnetic films in almost perfect agreement to FMR experiments as I will show. A striking feature e.g. is the mode splitting due to the two-magnon scattering which opens magnonic band gaps. This splitting can be tailored by the geometric and magnetic sample parameters.

This work was supported by the DFG grants FA 314/6-1, FA314/3-2.

[1] P. Landeros and D. L. Mills, Phys. Rev. B 85, 054424 (2012).

Topical Talk DS 25.4 Wed 16:30 H10

Gilbert damping parameter from first-principles — •Diemo Ködderitzsch[1], Sergiy Mankovsky[1], Hubert Ebert[1], and Georg Woltersdorf[2] — [1]Universität München, Dept. Chemie, Butenandtstraße 5-13, D-81377 München, Germany — [2]Universität Regensburg, Fak. f. Physik, Universitätsstraße 31, 93040 Regensburg, Germany

Conventionally, magnetisation dynamics is discussed on the basis of the Landau-Lifshitz-Gilbert equation containing a damping term for the magnetisation. So far in first-principles calculations, the scattering processes responsible for the transfer of energy associated with the magnetisation to the lattice (due to spin-orbit coupling) are usually represented by an adjustable relaxation time parameter. Recent approaches tackled this problem by introducing a scheme employing scattering theory. [1,2] We here present a general approach to calculate the damping parameter from first-principles based on the linear response Kubo formalism, as implemented within the fully relativistic Korringa-Kohn-Rostoker band structure method. This approach allows, in particular, to account for scattering processes due to chemical disorder or thermal lattice vibrations. Results for $3d$ transition-metals and their alloys, and impurity systems, compared to experiment demonstrate the viability of the approach. [3,4]

[1] Brataas *et al.*, PRL **101**, 037207 (2008) [2] Starikov *et al.*, PRL **105**, 236601 (2010) [3] Ebert, Mankowsky, Ködderitzsch and Kelly, PRL **107**, 066603 (2011) [4] Mankowsky, Ködderitzsch, Woltersdorf and Ebert, submitted to PRB (2012)

Topical Talk DS 25.5 Wed 17:00 H10

Spin dynamics and relaxation in ferrimagnets — Frank Schlickeiser, Sönke Wienholdt, Denise Hinzke, and •Ulrich Nowak — Universität Konstanz, 78457 Konstanz, Germany

Recent experiments on all-optical switching in GdFeCo [1] have focused much attention on the spin dynamics of ferrimagnets. The understanding of relaxation mechanisms is here even more complicated than in a ferromagnet due to the fact that the two sublattices of the ferrimagnet can exchange energy and angular momentum without dissipation, keeping the total energy and angular momentum constant.

We discuss the theory of the dynamics of ferrimagnets on different length scales, ranging from microscopic spin models to mesoscopic descriptions with a two-sublattice Landau-Lifshitz-Bloch equation. Our results for the temperature dependence of the frequencies and effective damping parameters of the normal modes represent a generalization and improvement of formetwo-sublatticer approximated solutions [2]. Furthermore, we discuss the role of angular momentum conservation and dissipation for the recently discovered transient ferromagnetic-like state [3] and for the pure thermal switching of ferrimagnets [4].

This work received funding from the EC (Collaborative Project FEMTOSPIN) and from the CAP at the University of Konstanz.

[1] K. Vahaplar *et al.*, Phys. Rev. Lett. **103**, 117201 (2009).
[2] F. Schlickeiser *et al.*, Phys. Rev. B, in press.
[3] I. Radu *et al.*, Nature **472**, 205 (2011).
[4] T. A. Ostler *et al.*, Nat. Commun. **3**, 666 (2012).

DS 26: Organic Electronics and Photovoltaics (jointly with CPP, HL, O)

Time: Wednesday 16:00–19:00 Location: H33

DS 26.1 Wed 16:00 H33

Effects of nuclear dynamics on light absorption, charge injection, recombination, and dye regeneration conditions in dye-sensitized solar cells — •Sergei Manzhos[1], Hiroshi Segawa[2], and Koichi Yamashita[3] — [1]Department of Mechanical Engineering, National University of Singapore, Blk EA #07-08, Singapore 117576 — [2]RCAST, University of Tokyo, 4-6-1, Komaba, Meguro-ku, Tokyo 153-8904, Japan — [3]Department of Chemical System Engineering, University of Tokyo, 7-3-1, Hongo, Bunkyo-ku, Tokyo 113-8656, Japan

We present molecular dynamics studies of effects of nuclear motions on light absorption and charge injection, recombination, and dye regeneration conditions for two organic dyes adsorbed on anatase (101) surface of TiO2 in mono- and bi-dentate configurations. We studied the effects of temperature, deuteration, and co-adsorbed water. Averaged over nuclear motions driving forces for injection and regeneration can differ significantly from their static estimates computed in most works. As a result, injection rate could be different by orders of magnitude. As the expectation value of the ground state energy is higher than its optimum geometry value (by up to 0.1 eV), nuclear motions will affect dye regeneration by recently proposed redox shuttle-dye combinations operating at low driving forces. Dye orientation motions are predicted to increase back-donation rate by orders of magnitude. Dye structure, adsorption mode, and the presence of water affect strongly the dynamics of energy level matching. Temperature in the range of 300-350K and deuteration have little effect on driving forces but red-shift of the absorption spectrum by a few %.

DS 26.2 Wed 16:15 H33

Photoemission Studies of Highly Reactive Organic Photosensitizers — •Mathias Fingerle[1], Maximilian Hemgesberg[2], Yvonne Schmitt[2], Sebastian Schmitt[2], Dimitri Imanbaew[2], Harald Kelm[2], Eugen Risto[2], Stefan Lach[1], Markus Gerhards[2], Christoph van Wüllen[2], Werner Thiel[2], and Christiane Ziegler[1] — [1]Fachbereich Physik, Erwin-Schrödinger-Str. 56, D-67663 Kaiserslautern, Germany — [2]Fachbereich Chemie, Erwin-Schrödinger-Str. 52, D-67663 Kaiserslautern, Germany

Substituted phenothiazines (PTs) are promising candidates for applications in the field of organic electronics. Due to the fact, that the electronic, magnetic and geometrical properties of the phenothiazine compared to its radical cation differ substantially, PT redox couples are of great interest for organic devices like dye sensitized solar cells (DSSCs). Here, the electronic properties of N-substituted phenothiazine dyes derived from 3.8-dithien-2-ylphenothiazine (DTPT), among them the first PT containing an olefinic moiety with an electron withdrawing group close to the nitrogen atom, were probed via photoemission spectroscopy. The thin film growth of the dyes and their oxidized species after spin coating was analyzed by X-ray photoelectron spectroscopy (XPS) and qualitatively visualized by scanning force microscopy (SFM). Through UV-photoelectron spectroscopy (UPS) and inverse photoelectron spectroscopy (IPES), the occupied and unoccupied energy levels could be attained and compared to data acquired by UV/Vis spectroscopy and DFT calculations. It is shown, that chemical oxidation by NOBF4 leads to a dramatic decrease of the band gap.

DS 26.3 Wed 16:30 H33

Investigation of the electronic structure of phosphorescent Platinum(II) complexes on Au(111) by STM and STS — •Pascal Raphael Ewen, Hasmik Harutyunyan, Jan Sanning, Matteo Mauro, Cristian Alejandro Strassert, and Daniel Wegner — Physikalisches Institut - Westfälische Wilhelms Universität Münster

Quenching effects still limit the efficiency of state-of-the-art organic light emitting diodes (OLEDs) at higher doping concentrations of the triplet emitter molecules within the emission layer. A possible candidate for avoiding of the loss of luminescence are recently synthesized Pt(II) complexes that do not show quenching even when aggregated into fibers or gels. The efficient implementation of such complexes in electronic devices requires a fundamental understanding of the interaction of the molecules with the local environment. A systematic investigation of the adsorption and the electronic structure of slightly different phosphorescent Pt(II) complexes offers information about the influence of ligands and substituents on the complexes as well as their interactions with neighbours and the substrate. We have studied the impact of molecule-surface and intermolecular interactions on the self-assembly and electronic structure of Pt-complex monolayers on Au(111) using scanning tunneling microscopy (STM) and spectroscopy (STS) at low temperature. By determining energies and spatial distributions of several frontier orbitals, we are able to evaluate the impact of hybridization on the molecular electronic structure with important consequences for the optical properties.

DS 26.4 Wed 16:45 H33

Overcoming the limitations of work-function modifications induced by adsorption of self-assembled monolayers — •Oliver T. Hofmann, Yong Xu, Patrick Rinke, and Matthias Scheffler — Fritz-Haber Institut der MPG, Berlin, Germany

Controlling the work function of electrodes critically determines charge-injection barriers and is of high importance for organic electronic devices. Such control can be easily achieved by adsorbing dipolar self-assembled monolayers. Despite the common application of this method, its limitations remain largely unexplored. It has, however, been demonstrated that charge-transfer occurs as soon as the molecular LUMO comes into resonance with the Fermi-energy when the molecular dipole moment is systematically increased by adding multiple repeat units. This Fermi-level pinning limits the achievable work-function modification. In turn, we argue that molecules with negative electron affinities never reach this limit and can reduce the work-function in principle all the way down to zero. As a proof of concept, we study the interaction between the ZnO($10\bar{1}0$) surface and pyridine using hybrid density functional theory with a variable fraction of exact exchange and a correction scheme for screened van-der-Waals forces. In agreement with experimental observations, we find an adsorption-induced work-function reduction of up to -2.9 eV. For a hypothetical ultra-dense pyridine monolayer the work-function reduction could even reach -4.3 eV for this surface.

DS 26.5 Wed 17:00 H33

Surface electronic structure and electron dynamics for pristine and adsorbate-covered ZnO($10\bar{1}0$) — •Jan-Christoph Deinert, Daniel Wegkamp, Michael Meyer, Julia Stähler, and Martin Wolf — Fritz-Haber-Institut der MPG, Abt. Physikalische Chemie, Faradayweg 4-6, 14195 Berlin

Zinc oxide is a promising electrode material for organic optoelectronics, because of its large optical band gap, possible n-type conductivity and its abundance. Despite many years of research, the electronic structure of interfaces between ZnO and - possibly functional - molecules or even its vacuum interface are not well understood. We use femtosecond time- and angle-resolved two-photon photoemission spectroscopy (2PPE) to analyze both the occupied and *un*occupied electronic states and dynamics at such interfaces. We show that hydrogen adsorption, even for very low coverage, leads to the formation of a surface electron accumulation layer and thus surface metallicity. Above band gap excitation with 3.8 eV fs laser pulses leads to ultrafast relaxation of hot electrons in the ZnO(10$\bar{1}$0) conduction band and the alleged formation of an excitonic state with a lifetime in the 100 ps range. Furthermore, we demonstrate that molecules with negative electron affinity allow for massive work function reduction of ZnO(10$\bar{1}$0), e. g. by $\Delta\Phi = -2.9$ eV in the case of a monolayer of pyridine. This opens a pathway to the design of cathodes with optimal electron injection barriers. We furthermore examine the changes in interfacial electronic structure upon biphenyl adsorption, which serves as a model system for optoelectronically functional poly(*p*-phenylene)-type molecules.

DS 26.6 Wed 17:15 H33

Defect-Driven Interfacial Electronic Structure at a Hybrid Organic / Inorganic Heterojunction — •Oliver Monti[1], Leah Kelly[1], Laura Schirra[1], Paul Winget[2], Hong Li[2], and Jean-Luc Bredas[2] — [1]The University of Arizona, Tucson, AZ, USA — [2]Georgia Institute of Technology, Atlanta, GA, USA

We present a combined experimental and theoretical study of the interfacial electronic structure of highly defined thin films of organic semiconductors on ZnO. We discuss the importance of shallow donor states in the near-surface region of ZnO in determining energy-level alignment and electronic structure at such interfaces. Using ultraviolet and x-ray photoelectron spectroscopy together with two-photon photoemission and first-principles calculations we investigate the nature of hybrid interface states inside the bandgap of ZnO. These states display strong charge-transfer character and may play an important role in charge-harvesting events in organic photovoltaic cells.

DS 26.7 Wed 17:30 H33

Electronic structure and excited states dynamics in polythiophene — •Lea Bogner[1], Gaurav Gupta[2], Michael Sommer[3], Mukundan Thelakkat[4], Thomas Thurn-Albrecht[2], and Petra Tegeder[1,5] — [1]Freie Universität Berlin, Fachbereich Physik — [2]Martin-Luther-Universität Halle-Wittenberg, Institut für Physik — [3]Albert-Ludwigs-Universität Freiburg, Institut für Makromolekulare Chemie — [4]Universität Bayreuth, Makromolekulare Chemie I — [5]Rubrecht-Karls-Universität Heidelberg, Physikalisch-Chemisches Institut

Semiconducting conjugated polymers exhibit promising properties for applications in optoelectronic devices such as organic photovoltaic cells. Poly(3-hexylthiophene) (P3HT) and other poly- and oligothiophenes are auspicious electron donor materials due to their high charge carrier mobility. In this study thin films of semi crystalline P3HT with different degree of crystallinity [1] have been investigated by means of time- and angle-resolved two-photon photoemission (2PPE). We observed several unoccupied and occupied electronic states (bands) including the valence and conduction band. In addition two excited states are found which possess lifetimes in the order of hundred picoseconds.

Ref.: [1] Z. Wu, A. Petzold, T. Henze, T. Thurn-Albrecht, R. H. Lohwasser, M. Sommer, M. Thelakkat, Macromolecules, 2010, 43, 4646-4653.

DS 26.8 Wed 17:45 H33

Charge transfer at the interface between substituted pentacene nanorods and gold single crystals — •Sabine-Antonia Savu, Maria Benedetta Casu, and Thomas Chassé — Institute of Physical and Theoretical Chemistry, University of Tübingen, Tübingen, Germany

Pentacene is one of the most investigated organic molecules due to its successful application in organic electronics. Substitution in pentacene gives the opportunity to tailor the properties which are needed for applications; therefore it is necessary to investigate its influence on molecular aggregation and thin film formation. In particular, here we report our investigations on nanorods of three newly synthesized substituted pentacenes with different degrees of fluorination. We performed X-ray photoemission spectroscopy (XPS), near edge X-ray absorption fine structure (NEXAFS) spectroscopy, and atomic force microscopy (AFM) on nanorods deposited on Au(111) and Au(110) single crystals. XPS thickness dependent spectra in combination with NEXAFS investigations show that the screening of the core hole occurs via charge transfer from the metal to the molecule. In addition, the morphology of the nanorods has been investigated by using AFM, evaluating the nanorod characteristics also from a statistical point of view and taking the different degree of fluorination into account.

DS 26.9 Wed 18:00 H33

Photoemission Investigation of the Electronic Structure of P3HT:PCBM Bulk-Heterojunctions using a lift-off technique — •Angela Eckstein[1,2], Dirk Hauschild[1,2], Julia Kern[3], Markus Mingebach[3], Carsten Deibel[3], Vladimir Dyakonov[3], Achim Schöll[1,2], and Friedrich Reinert[1,2] — [1]Experimentelle Physik VII, Universität Würzburg, 97074 Würzburg — [2]Gemeinschaftslabor für Nanoanalytik, Karlsruher Institut für Technologie KIT, 76021 Karlsruhe — [3]Experimentelle Physik VI, Universität Würzburg, 97074 Würzburg

Poly(3-hexylthiophene): phenyl-[6,6]-C61 butyric acid methyl ester (P3HT:PCBM) bulk heterojunctions (BHJ) are prototype active layers for organic solar cells. The electronic structure at the internal interface can be accessed by photoelectron spectroscopy (PES), thus providing insight into the alignment of the electronic levels and the occurrence of possible interface dipoles. However, the very surface sensitive PES investigation is complicated in case of P3HT:PCBM bulk heterojunctions since the film preparation by spin-coating creates a P3HT wetting layer on the film surface. In order to avoid this problem we used a lift-off technique to access the interface to the spin coating substrate (SiO2), which has shown to resemble the bulk situation [1]. P3HT:PCBM samples with different mixing ratio, which can be lift-off-prepared under UHV-condition thus avoiding contamination by ambient conditions, have been investigated by x-ray- and UV-PES as well as by inverse PES with particular respect to the influence of degradation and radiation damage. [1] Kahn et al. (Org. El. 11 (2010) 1779-1785)

DS 26.10 Wed 18:15 H33

Bottom-up synthesis of self-aligned conjugated polymers — Sören Krotzky[1], •Rico Gutzler[1], Vijay Vyas[1,2], Bettina Lotsch[1,2], and Klaus Kern[1,3] — [1]Max Planck Institute for Solid State Research, Stuttgart, Germany — [2]Department of Chemistry, University of Munich (LMU), Munich, Germany — [3]Institut de Physique de la Matière Condensée, Ecole Polytechnique Fédérale de Lausanne, Switzerland

We investigate the synthesis of self-assembled organometallic structures and well-defined long 1D polymers by the surface-supported Ullmann reaction on an Ag(111) surface. The brominated semiconducting precursor molecule (2,7-dibromobenzothieno[3,2-b]benzothiophene) is sublimed under UHV conditions on the crystalline surface where a dehalogenation step is induced at room temperature. STM reveals self-assembly of the dehalogenated ditopic molecule into short organometallic coordination polymers that arrange in a ladder-like monolayer. Annealing to 420 K leads to C-C coupling of the molecules via ejection of the coordinated metal atom. At this temperature the newly formed 1D polymer strands align in a side-by-side manner with three preferred directions with respect to the high-symmetry directions of the surface. DFT calculations show that the length of the synthesized polymers is sufficient to reduce the HOMO-LUMO gap to its value at infinite length of the polymer. Together with the calculated band-structure this suggests possible unidirectional charge mobility within the well-ordered semiconducting polymeric monolayer.

DS 26.11 Wed 18:30 H33

How contact groups influence metal molecule hybrid structures under voltage — •Simon Liebing, Torsten Hahn, and Jens Kortus — TU Bergakademie Freiberg, Freiberg, Germany

In order to use molecules in electronics it is not only important to understand the properties of molecules themself but also properties of metal-molecule interfaces. Recent contributions discussed the behavior of thiole [1] and amino linker groups [2]. To get a more systematic understanding the authors have chosen a model system of benzene with variable linker groups between gold electrodes. Such groups can be thiole, amino, thiophen, nitrile, pyrol and cyanide. This allows for example to study the differences between σ- and π- like symmetry with respect to the individual interface geometry. The theoretical study combines the calculation of single molecule properties by density functional theory [3] with the nonequilibrium Greens functions technique [4] to calculate the transport properties [5] of the device. [1] Markussen, T. et al. JCP **132** , 224104 (2010)

[2] Angela, D. et. al. Nano Letters **10**, no. 7 (2010)

[3] Pederson, M. et. al. Phys. Status Solidi b **217**, 197. (2000)

[4] Datta, S. Nanotechnology **15**, 433. (2004)

[5] Brandbyge, M. Phys. Rev. B **65**, 165401 (2002)

DS 26.12 Wed 18:45 H33

Improving the contact materials of organic electronic devices: Polymeric dipole layers vs. self assembling monolayers — •Janusz Schinke[1,2], Julian Heusser[3,2], Marc Hänsel[3,2], Julia Maibach[4,2], Wolgang Kowalsky[1,2], Michael Kröger[1,2], Eric Mankel[4,2], and Wolfram Jaegermann[4,2] — [1]TU Braunschweig, Institut für Hochfrequenztechnik — [2]Innovation Lab GmbH — [3]Universität Heidelberg, Kirchhoff-Institut für Physik — [4]TU Darmstadt, Materials Science Institute, Surface Science Division

In organic electronic devices, charge injection at the contacts is crucial for high electrical performance. Most of these devices require at least one electrode with a sufficiently low work function (WF). Low-WF electrodes like alkaline earth metals are easily available; however, they are chemically very reactive and oxidize in ambient atmosphere. A smart way to overcome this problem is the use of molecular or polymeric dipole layers (PDLs). The use of PDLs to tune an electrodes work function can be advantageous over self assembled monolayers(SAMs) as the PDL concept can be applied to a wider range of electrode materials like ITO, Ag, Au or Al. We have used two different PDLs: branched polyethylenimine (PEI) and polyethyleneimine ethoxylate (PEIE). We studied the the properties of PDL treated substrates via AFM, ambient Kelvin probe and XPS/UPS. Both interlayers lower the metal substrate work function by approx. 1000meV. On ITO we reach absolute values of about 3.0eV which leads to strongly enhanced electron injection in model devices.

DS 27: Thin Film Characterization: Structure Analysis and Composition (XRD, TEM, XPS, SIMS, RBS,...) I

Time: Wednesday 17:15–19:45 Location: H32

DS 27.1 Wed 17:15 H32

In-situ GISAXS study of the gold electrode growth on spiro-OMeTAD films — •Martin A. Niedermeier[1], Ezzeldin Metwalli[1], Volker Körstgens[1], Jan Perlich[2], Ralf Röhlsberger[2], Stephan V. Roth[2], and Peter Müller-Buschbaum[1] — [1]TU München, Physik Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching, Germany — [2]HASYLAB at DESY, Notkestraße 85, 22603 Hamburg, Germany

In the fast developing field of organic electronics, thin metal films play a huge role as they are commonly applied as electrode materials. One prominent example is the field of photovoltaics which has taken on greater significance in the recent years due the energy challenges of modern society. A well-defined organic/metal interface is crucial for a good overall device performance. For a profound understanding of that interface, the morphology and the incorporation of the electrode material into the organic film is essential. However, so far only little fundamental knowledge is available on this topic.

In this work, we present an in-situ investigation of the gold electrode growth via sputter deposition on top of a spiro-OMeTAD film, which is a commonly used system in solid-state dye sensitized solar cells. We used grazing incidence small angle x-ray scattering (GISAXS) with high time resolution to follow the real time evolution of the gold electrode growth and obtain information about the growth kinetics. Additionally, enrichment layers of gold into the organic film are investigated with x-ray reflectivity. Therefore, we obtain a good fundamental understanding of the electrode/organic semiconductor interface.

DS 27.2 Wed 17:30 H32

Gold Cluster Growth Kinetics during Sputter Deposition — •Matthias Schwartzkopf[1], Adeline Buffet[1], Volker Körstgens[2], Ezzeldin Metwalli[2], Kai Schlage[2], André Rothkirch[1], Monika Rawolle[2], Jan Perlich[1], Gerd Herzog[1], Berit Heidmann[1], Ralf Röhlsberger[1], Peter Müller-Buschbaum[2], Rainer Gehrke[1], and Stephan V. Roth[1] — [1]DESY, Notkestr. 85, D-22607 Hamburg, Germany — [2]TU München, James-Franck-Str. 1, D-85747 Garching, Germany

The adjustment of size-dependent catalytic, electrical and optical properties of gold cluster assemblies is a very significant issue in modern applied nanotechnology. We investigate in situ the growth kinetics of gold nanostructures to a gold layer during magnetron sputter deposition with high time resolution by means of grazing incidence small-angle X-ray scattering (GISAXS). The high time resolution in the millisecond regime allows the determination of kinetics of initial nucleation and subsequent cluster growth during sputter deposition at deposition rates relevant for industrial manufacturing processes. Morphological parameters related to the growth of metallic layers such as cluster size, correlation distance and surface coverage are deduced from a general model solely based on geometrical assumptions. The temporal evolution of the model parameters reveals four stages of gold cluster growth, namely initial nucleation, diffusion-mediated coalescence, adsorption-driven cluster growth and finally grain growth above the percolation threshold. Furthermore, our study opens up the opportunity to deduce the wetting behaviour of gold nanoclusters on solid substrates.

DS 27.3 Wed 17:45 H32

Growth kinetics of metal nanoparticles on polymer surfaces — •Ezzeldin Metwalli[1], Volker Körstgens[1], Adeline Buffet[2], Jan Perlich[2], Stephan V. Roth[2], and Peter Müller-Buschbaum[1] — [1]TU München, LS für Funktionelle Materialien, Physik-Department, James-Franck-Str. 1, 85747 Garching, Germany — [2]HASYLAB at DESY, Notkestr. 85, 22603 Hamburg, Germany

Metal layers on polymer films [1-4] are essential for many important nanodevices such as organic solar cells and light emitting diodes. Gold in its atomic state is deposited on several homopolymer and block copolymer films by utilizing a DC magnetron sputtering deposition system. With the unprecedented time resolution of 15 milliseconds, the nucleation/growth kinetics of gold nanoparticles on the polymer surfaces is monitored using in situ real-time grazing incidence small angle x-ray scattering (GISAXS) technique. An exponential growth of metal particle size on all polymer surfaces is observed prior to the formation of a quasi uniform metal layer. Below a certain critical particle size, an initial fast particle growth is due to high particle mobility. While a slower kinetics at concentrated metal dispersion is due to the strong metal-metal interactions. This novel kinetic study of metal growth on chemically different homopolymer films clearly explains the high selectivity characteristics of metals towards a particular block of diblock copolymer nanotemplates. 1. E.Metwalli et al. Langmuir 24, 4265 (2008) 2. E.Metwalli et al. Langmuir 25, 11815 (2009) 3. G.Kaune, E.Metwalli et al. ACS Appl. Mater. Interfaces 3, 1055 (2011) 4. X.Xia, E.Metwalli, et al. J. Phys. Condens. Matter 23, 254203 (2011)

DS 27.4 Wed 18:00 H32

In situ GISAXS characterization of Al sputtering on Alq3 thin film — •Shun Yu, Gonzalo Santoro, Jan Perlich, Marion Kuhlmann, Johannes F.H. Risch, Matthias Schwartzkopf, and Stephan V. Roth — HASYLAB, DESY, Notkestraße 85, 22607, Hamburg

Organic light emitting diode (OLED) is an important device as the next generation light source for illumination. Its low cost, easy fabrication and relatively high efficiency have attracted many research interests. The multilayer device structure emphasizes the significance of understanding the interfacial structure and properties. In most OLEDs, Al is used as the metal electrical contact and Tris(8-hydroxyquinolinato)aluminium (Alq3) is the activating layer. Upon sputtering on Alq3, Al can diffuse into the organic layer, modifying both the morphological and electronic structures and consequently the device performance. The interaction between Al and Alq3 has been studied by different spectroscopic techniques and theoretical methods at single molecule level. Nevertheless, the growth of the Al thin film on Alq3 is scarcely studied. In this work, we have exploited in situ grazing incident small angle X-ray scattering (GISAXS) technique to monitor the growth of Al thin film on top of Alq3 layer during the high speed sputtering process in real time. As a result, we elucidate three growing stages from the out-of-plane scattering pattern. Meanwhile, both Al and Alq3 films demonstrate good correlation to substrate roughness. The results benefit the comprehension of the general industrial sputtering process.

DS 27.5 Wed 18:15 H32

In situ study of the texture development during the growth of magnetron sputtered VC thin films

— •Sunil Kotapati[1], Bärbel Krause[1], Marthe Kaufholz[1], Stephen Doyle[2], Miguel Mantilla[3], Michael Stüber[4], Sven Ulrich[4], and Tilo Baumbach[1,2] — [1]Institut für Photonenforschung und Synchrotronstrahlung, KIT, Germany — [2]ANKA, KIT, Germany — [3]Max-Planck-Institut für Intelligente Systeme, Stuttgart, Germany — [4]Institut für Angewandte Materialien - Angewandte Werkstoffphysik, KIT, Germany

Hard coatings deposited by magnetron sputtering play a major role in enhancing the lifetime of machining tools and maintaining their productivity. In situ x-ray experiments during thin film deposition are an extremely useful tool to understand the interplay between the microstructure and macroscopic coating properties. The aim of this study is to develop a model for the structure formation of hard coatings as a function of different process parameters such as growth temperature and bias. For this, several Vanadium carbide (VC1-x) thin films were deposited at different growth conditions. In addition to in situ X-ray powder diffraction, the complementary ex situ methods AFM and TEM were used. The powder rings obtained during deposition reveal that below a transition temperature T~250°C, a mixture of [111] and [200] textures dominates, while the preferred [111] orientation is found above T. The real time measurements also show that there are structural changes as a function of deposition time.

DS 27.6 Wed 18:30 H32

In situ control of the structure formation of PVD hard coatings: periodic modulation of the microstructure

— •Marthe Kaufholz[1], Bärbel Krause[1], Sunil Kotapati[1], Michael Stueber[2], Sven Ulrich[2], Miguel Mantilla[3], and Tilo Baumbach[1,4] — [1]IPS, KIT, Germany — [2]IAM-AWP,KIT,Germany — [3]MPI for Intelligent Systems, Germany — [4]ANKA, KIT, Germany

Hard coatings such as Vanadium Carbide (VC_{1-x}) are nowadays commonly used for improving the life-time of tools. Multilayer systems are one way to enhance the hardness of such coatings. They usually consist of alternating layers of two different materials.

In situ X-ray Reflectivity measurements at the synchrotron ANKA and ex situ Transmission Electron Microscopy studies showed that the density of thin VC_{1-x} films depends on the sputtering conditions. A two layer system with different densities could be grown by varying the gas flow of the sputter gas.

By repeating this process periodically, a multilayer system was successfully created. Such a multilayer system formed by only one material simplifies the synthesis process and is of great interest for optical applications.

DS 27.7 Wed 18:45 H32

X-ray Grazing Incidence Diffraction from OTS-SAMs on Metal Oxides

— •Hans-Georg Steinrück[1], Stefan Gerth[1], Michael Klimczak[1], Moshe Deutsch[2], Ben Ocko[3], and Andreas Magerl[1] — [1]Lehrstuhl für Kristallographie und Strukturphysik, Universität Erlangen Nürnberg , Germany — [2]Bar-Ilan University, Ramat-Gan, Israel — [3]Brookhaven National Laboratory, Upton NY, USA

We investigated the in-plane structural properties of octadecyltrichlorosilane ($C_{17}H_{37}Cl_3Si$, OTS) self-assembled monolayers on amorphous SiO_2, quartz (001) and sapphire (001) via X-ray grazing incident diffraction.

For all three systems a powder like diffraction ring at $\mathbf{q}_r = 1.50Å^{-1}$ was found. The radial width of these peaks corresponds to a coherence length of about 4 OTS molecular diameters, which fits well with the findings of Tidwell et al. for OTS monolayers on amorphous SiO_2 [1].

For OTS on sapphire the azimuthal scans show increasing peak intensities towards the sapphire in-plane peak, suggesting orientational order of the OTS film which is likely related to the good lattice match with the sapphire. This epitaxial behavior depends on the headgroup properties of hydrocarbon chain monolayers, as Ocko et al. have shown perfect commensurabiltiy for $C_{18}H_{37}OH$ on sapphire [2].

Further the temperature dependence of the lateral structure was investigated yielding a decreasing intensity and an increasing lattice spacing with increasing temperature for all three systems.

[1] Tidswell et al., J. Chem. Phys. 95, 2854 (1991)
[2] Ocko et al., Phys. Rev. Lett. 106, 137801 (2011)

DS 27.8 Wed 19:00 H32

Sol-Gel Type $Ga_{2-x}Fe_xO_3$ Thin Films: Towards Room Temperature Magnetic Oxides with an Ordered Mesoporous Morphology and Nanocrystalline Wall Structure

— •Christian Reitz, Christian Suchomski, Robert Kruk, and Torsten Brezesinski — Institute of Nanotechnology (INT), Karlsruhe Institute of Technology (KIT), 76344 Eggenstein-Leopoldshafen

Both ferri(o)magnetism and ferroelectricity are indispensable in modern technologies and have been used in devices for quite some time. To further increase the performance, the materials employed need to be reduced to the nanometer scale. The same principle also pertains to multiferroics, showing coupling of both magnetic and electric order parameters. Such materials hold great promise for many applications. Among the few single-phase multiferroics that have been discovered to date, $Ga_{2-x}Fe_xO_3$ (GFO) has recently been receiving increasing attention. In this work we focus on ordered large-pore mesoporous GFO thin films with nanocrystalline walls. These materials were produced through facile polymer templating strategies and served as model systems to obtain a better understanding of the relationships between nanoscale structure and ferroic properties. Electron microscopy, GISAXS, XPS, Raman spectroscopy and magnetization and Mössbauer studies confirmed the high-quality of the sol-gel derived thin films with ferrimagnetic ordering at room temperature and provided insight into the underlying coupling phenomena. At this point, it is envisioned that the pore cavities will facilitate the fabrication of novel magnetically exchange-coupled composites.

DS 27.9 Wed 19:15 H32

Depth dependent influence of thin Fe layers on the magnetic properties of Pd in Pd/Fe multilayers

— •Paul Zakalek, Markus Schmitz, Ulrich Rücker, and Thomas Brückel — Jülich Centre for Neutron Science JCNS und Peter Grünberg Institut PGI, Forschungszentrum Jülich GmbH, D-52425 Jülich, Germany

Proximity effects in magnetic multilayers give rise to new physical properties which are interesting for new spintronic devices. Because of a high Stoner parameter of 0.78, Pd almost fulfills the Stoner-criterion for ferromagnetism and makes this material especially interesting. Due to hybridization with a magnetic material like Fe it is possible to induce a magnetic moment into the Pd layer.

Therefore we investigated Pd/Fe multilayers with sharp defined interfaces (layer roughnesses of less then 8 Å) with SQUID magnetometry, X-ray and polarized neutron reflectrometry measurements. The SQUID measurements could indicate an existing induced magnetic moment of Pd, which was not possible to resolve with polarized neutron reflectrometry measurements.

We will present the preparation and characterization of the Pd/Fe multilayers.

DS 27.10 Wed 19:30 H32

Formation of supersaturated AuNi nanoparticles via solid state dewetting of Au/Ni thin bilayers

— •Andreas Herz, Dong Wang, and Peter Schaaf — Institut für Werkstofftechnik, Fachgebiet Werkstoffe der Elektrotechnik, Ilmenau, Germany

Thin films undergo agglomeration upon annealing due to their high surface-to-volume ratio which produces a large driving force for reduction of surface area. This process is known as dewetting and can occur well below the melting temperature of the layer material. In recent years, dewetting of thin metal films has therefore become a promising method for fabricating various nanostructures with potential applications in catalysis, plasmonics, or magnetic devices. However, nanoalloys may reveal new or even unique properties due to the combination of size and composition. Thus, thin bilayer systems consisting of a pair of metals, e.g. Au and Ni, could be a convenient basis for the self-organized synthesis of novel alloy nanostructures via dewetting.

DS 28: Layer Properties: Electrical, Optical, and Mechanical Properties

Time: Thursday 9:30–13:00 Location: H8

DS 28.1 Thu 9:30 H8

Crystallization Kinetics of Phase-Change Materials in the High-Speed Regime — •Julia Benke[1], Egidio Carria[1], Martin Salinga[1,2], and Matthias Wuttig[1,2] — [1]I. Physikalisches Institut (IA) — [2]JARA-FIT, RWTH Aachen

Phase-change materials (PCM) are dominating the field of rewritable optical data storage. The pronounced optical contrast between their amorphous and crystalline phase is used to code the digital information in rewritable CDs, DVDs and Blue-Ray discs. Nevertheless these devices do not tap the full potential of PCM. The fast transition between the two phases can compete with writing speed in DDR-RAM and, atdditionally, this technology provides the great advantage of non-volatility.

In recent years, many efforts have been spent to unravel the origin of the ultra-fast phase transition. Especially, the limiting process of crystallization has attracted much interest. PCMs can be divided into two classes, nucleation-dominated materials like Ge2Sb2Te5 and growth-dominated materials such as Ag-In-doped Sb2Te. The interplay of nucleation and growth during the crystallization process is of great interest for the reliability of down-scaled PC-memory cells. With our new Phase-change Optical Tester, we have investigated the crystallization kinetics of GeTe and Ag-In-doped Sb2Te under isothermal conditions over a large temperature range up into the high-speed regime. Starting from these measurements, we have inferred several properties of the melt-quenched amorphous phase building a general correlation with the switching mechanism in PCMs.

DS 28.2 Thu 9:45 H8

(Magneto)-optical investigations of $NiFe_2O_4$ and $CoFe_2O_4$ epitaxial thin films — •Cameliu Himcinschi[1], Ionela Vrejoiu[2,4], Georgeta Salvan[3], Michael Fronk[3], Andreas Talkenberger[1], Dietrich Zahn[3], and Jens Kortus[1] — [1]TU Bergakademie Freiberg, Institute of Theoretical Physics, D-09596 Freiberg — [2]Max Planck Institute of Microstructure Physics, Weinberg 2, D-06120 Halle — [3]TU Chemnitz, Semiconductor Physics, D-09107 Chemnitz — [4]Max Planck Institute for Solid State Research, D-70569 Stuttgart

Nickel and cobalt ferrite epitaxial films were deposited on Nb doped $SrTiO_3$ by pulsed laser deposition. X-Ray diffraction and atomic force microscopy showed that the films have a good crystalline quality and smooth surfaces. A larger number of phonons was observed in the polarization dependent Raman spectra of the ferrite films than expected for the cubic spinel structures. This is explained by short range ordering of the Ni^{2+}(or Co^{2+}) and Fe^{3+} cations at the octahedral sites inducing a lowering of the symmetry. The dielectric functions for nickel and cobalt ferrites are determined from ellipsometry in the 0.73-5eV photon energy range. The absorption edge was analyzed using a bandgap model and the energies for the indirect and direct optical transitions were calculated. Magneto-optical Kerr effect spectroscopy in combination with spectroscopic ellipsometry allowed the off-diagonal elements of the dielectric tensor to be determined in the energy range from 1.7 eV to 5eV.

DS 28.3 Thu 10:00 H8

Superconductivity in the turbostratically disordered misfit layered compounds $[(PbSe)_{1.10}]_m(NbSe_2)_n$ — •Corinna Grosse[1], Zachary Jones[2], Olivio Chiatti[1], Matti Alemayehu[2], David C. Johnson[2], and Saskia F. Fischer[1] — [1]Novel Materials, Humboldt-Universität zu Berlin, 10099 Berlin, Germany — [2]Department of Chemistry, University of Oregon, Eugene, OR 97401-3753, USA

The turbostratically disordered $[(PbSe)_{1.10}]_m(NbSe_2)_n$ misfit layered compounds, so called *ferecrystals*, are novel materials composed of alternatingly stacked superconductors and normal conductors. They allow us to study the effects of turbostratic disorder, layer thickness and stacking sequence on the electrical properties. Oosawa *et al.* [1] have observed superconductivity in $[(PbSe)_{1.10}]_m(NbSe_2)_n$ misfit layered compounds without turbostratically disordered structure. We carried out temperature-dependent in-plane resistivity measurements down to 300 mK on $[(PbSe)_{1.10}]_m(NbSe_2)_n$ ferecrystals as well as angle-dependent magnetotransport measurements and compare the results to the measurements in [1]. We observed resistive transitions to the superconducting state with critical temperatures below those reported in [1]. Critical currents were measured as a function of temperature for samples with different (m,n) values. Angle-dependent magnetoresistance measurements below T_c show that the in-plane resistance is anisotropic with regard to the direction of the external magnetic field.

[1] Y. Oosawa *et al.* Jpn. J. Appl. Phys. Vol. 31 (1992), L1096-L1099.

DS 28.4 Thu 10:15 H8

CVD-Like Growth Mechanism and 3D Nucleation in ZnO-TFTs Deposited by Pulsed Spray Pyrolysis — •Marlis Ortel and Veit Wagner — Research Center for Functional Materials and Nanomolecular Science, Jacobs University Bremen, Campus Ring 1, 28759 Bremen, Germany

Zinc oxide is a promising material for large area electronics due to high mobility and large area compatible deposition techniques. Proper film formation is crucial to obtain high quality layers. We investigate the growth and nucleation of zinc oxide thin films deposited by pulsed spray pyrolysis from aqueous zinc-precursor solution is investigated. The Leidenfrost effect was found to be a crucial mechanism during film growth since the Leidenfrost point has to be exceeded to form high quality layers. Furthermore, it is concluded that 3D nucleation of ZnO nano-crystals takes place out of the gaseous phase by a CVD-like process on ITO as well as on SiO2 substrates. Surface crystal orientation and roughness of the zinc oxide layer are found to be substrate dependent. These findings were utilized to optimize the deposition of the active layer in a zinc oxide thin film transistor (TFT) and investigate its semiconducting properties as degree of quality of the functional layer. Under optimized conditions the mobility was found to exceed 12cm2V-1s-1, the on-set was at 1V and the on-off current ratio was found to be higher than 108.

DS 28.5 Thu 10:30 H8

Modellierung des spektralen Reflexionsgrades verschiedener ITO Schichten nur mit Hilfe des Drude Modells — •Nadine Wolf, Daniel Gerstenlauer und Jochen Manara — Bayerisches Zentrum für Angewandte Energieforschung e.V., Würzburg

Um die Korrelation zwischen den elektrischen und den infrarot-optischen Eigenschaften von verschiedenen Zinn dotierten Indiumoxid (engl. tin doped indiumoxide, ITO) Schichten im infraroten Spektralbereich zu untersuchen, wurde der spektrale Reflexionsgrad vermessen und im nahen infraroten Spektralbereich analysiert. ITO stellt dabei das ideale Material dar um zu überprüfen, ob der gemessene Reflexionsgrad im NIR Bereich ausschließlich mit Hilfe des Drude Modells beschrieben werden kann, da die optischen und elektrischen Eigenschaften von ITO in erster Linie anhand der Freien-Elektronen-Theorie beschrieben werden können.

Die gemessenen spektralen Reflexionsgrade verschieden prozessierter ITO Schichten wurden anhand des Drude Modells gefittet, indem die Hochfrequenz-Dielektrizitätskonstante, die Streuzeit und der Quotient aus der Ladungsträgerdichte und der effektiven Masse der Elektronen über einen Least Square Fit angepasst wurden.

Es wird gezeigt, dass die erhaltenen Fitparameter konsistent sind, d.h. die Ladungsträgerdichte, die Streuzeit und die dielektrische Konstante der verschiedenen ITO Schichten verhalten sich zueinander wie erwartet und stimmen mit den Literaturwerten gut überein. Demzufolge ist es möglich die gemessenen Reflexionsgrade verschieden prozessierter ITO Schicht nur mit Hilfe der Drude Gleichungen zu fitten.

DS 28.6 Thu 10:45 H8

Transition levels of defects in $CuAlO_2$ — •Charles Patterson and Ciaran McNamee — School of Physics, Trinity College Dublin, Dublin 2, Ireland.

$CuAlO_2$ has been investigated as a potential p-type semiconducting oxide for transparent conducting oxide applications. The perfect crystal is a wide gap insulator and its p-type conductivity is believed to arise from V_{Cu} vacancy defects, which are abundant in $CuAlO_2$. We report calculations of defect formation energies and charge transition levels for V_{Cu}, V_O, V_{Al} vacancies, Cu_{Al} and Al_{Cu} substitutions and the Oi_i interstitial. Calculations are performed using a hybrid density functional theory (DFT) method. The electronic structure of each defect and charge state is investigated in detail. The V^-_{Cu}/V^0_{Cu} transition level is lower than that predicted in a previous hybrid DFT calculation and may be in better agreement with results from measurements of carrier density versus temperature in $CuAlO_2$.

DS 28.7 Thu 11:00 H8

Systematic investigations of low energy ion beam sputtering of Si and Ag — •René Feder, Frank Frost, Horst Neumann, Carsten Bundesmann, and Bernd Rauschenbach — Leibniz-Institut für Oberflächenmodifizierung e.V„ Permoserstr. 15, 04318 Leipzig, Germany

Ion beam sputter deposition (IBD) provides intrinsic features which influence the properties of the growing film, because ion properties and geometrical process conditions generate different energy and spatial distribution of the sputtered and scattered particles.

A vacuum deposition chamber has been set up which allows ion beam sputtering of different targets under variation of geometrical parameters and of ion beam parameters to make a systematic analysis of the correlation between the properties of the ion beam, the properties of the sputtered and scattered particles, and the properties of the deposited films. A set of samples was prepared and characterized with respect to selected film properties, such as thickness and surface topography. The experiments indicate a systematic influence of the deposition parameters on the film properties. Because of this influence, the energy distribution of secondary particles was measured using an energy-selective mass spectrometer. Among others, experiments revealed a high-energetic maximum for backscattered primary ions, which shifts with increasing emission angle to higher energies. Experimental data are compared with Monte Carlo simulations done with the well-known TRIM.SP code.

Financial support by DFG within project BU2625/1-1.

Coffee break (15 min)

DS 28.8 Thu 11:30 H8

Attenuation of coherent longitudinal acoustic phonons in free-standing gold-membranes — •Alexandra Frik[1], Mike Hettich[1], Oliver Ristow[1], Martin Grossmann[1], Axel Bruchhausen[2], Martin Schubert[1], and Thomas Dekorsy[1] — [1]Department of Physics and Center of Applied Photonics, University of Konstanz, 78457 Konstanz, Germany — [2]Instituto Balseiro & Centro Atomico Bariloche (CNEA), and CONICET, Argentina

The damping time of coherent longitudinal acoustic phonons in free standing gold membranes is measured by high speed asnchronous optical sampling (ASOPS) [1], a modified femtosecond pump probe spectroscopy method. We investigate the frequency dependence of the fundamental thickness mode lifetime by varying the membrane thickness. In addition, we study the influence of the surface roughness on the mode lifetimes. Temperature dependent measurements allow us to seperate the intrinsic damping mechanisms from surface contributions. The free-standing membranes were produced by thermal evaporating and where subsequently placed on a TEM-grid by a floating technique.

[1] A. Bartels Entwicklung von Femtosekundenlasern mit Repetitionsraten oberhalb 1 GHz und ihre Anwendungen Shaker Verlag Aachen, ISBN: 3-8265-8400-7 (2001)

DS 28.9 Thu 11:45 H8

Generation of a broadband acoustic frequency comb in the 100 GHz-range — •Martin Grossmann[1], Oliver Ristow[1], Mike Hettich[1], Chuan He[1], Reimar Waitz[1], Patricia Scheel[1], Axel Bruchhausen[2], Martin Schubert[1], Vitaly Gusev[3], Elke Scheer[1], and Thomas Dekorsy[1] — [1]Department of Physics, University of Konstanz, D-78467 Germany — [2]Instituto Balseiro & Centro Atómico Bariloche (CNEA), and CONICET, Argentina — [3]Institut des Molécules et Matériaux du Mans, UMR CNRS 6283, Université du Maine,France

Acoustic properties in the GHz frequency range are not very well understood for most semiconductors although intrinsic attenuation and scattering at interfaces of acoustic waves is of great interest for both fundamental and applied science. Additionally adhesion properties of very thin films are both hard to control and to evaluate. A thin Al/Si-membrane which is investigated by asynchronous optical sampling, a pump-probe technique, can be used to gain knowledge of these crucial properties. The cavity-like behavior for acoustic pulses of the membrane is used to generate a frequency comb in the 100 GHz range consisting of 24 eigenmodes. By analyzing the Fourier spectrum of the generated acoustic pulse we can evaluate the adhesion of the two layer system and by analyzing the individual reflected pulses, frequency dependent damping constants can be extracted for frequencies up to 300 GHz. Furthermore a frequency shift of the higher harmonics from the expected values given by the ground mode due to the two-layer system is measured.

DS 28.10 Thu 12:00 H8

Coherent phonon pump-probe spectroscopy on off-stoichiometric Co-doped NiMnGa films — •Martin Schubert[1], Jan Mayer[1], Mike Hettich[1], Hanjo Schäfer[1], Aleksej Laptev[1], Moritz Merklein[1], Chuan He[1], Martin Grossmann[1], Oliver Ristow[1], Yuansu Luo[2], Vitalyi Gusev[3], Jure Demsar[1], Mikhail Fonin[1], Konrad Samwer[1], and Thomas Dekorsy[1] — [1]Department of Physics, University of Konstanz, Germany — [2]Physikalisches Institut, Georg-August-Universität Göttingen, Germany — [3]Université du Maine, Le Mans, France

The shape memory alloy NiMnGa is characterized by a reversible and diffusionless structural transition from a high-temperature austenitic phase to a low-temperature martensitic phase, which can be induced by stress or temperature. We investigated the phase transition of off-stoichiometric NiMnGa thin films with and without Co-doping by asynchronous optical sampling (ASOPS), an ultra-fast optical pump-probe measurement technique. A wide range of different compositions is investigated by both cooling and/or heating the sample depending on the transition temperature. For all samples that were investigated, a distinct softening of the dominant acoustic phonon mode can be observed when the temperature of the sample approaches the phase transition temperature. Structural changes due to heating are not sufficient to explain the shift in frequencies. The softening is therefore linked to a strong electron-phonon interaction similar to that in a charge density wave (CDW) system. CDW haven't been observed in off-stoichiometric films but they have been measured in stoichiometric NiMnGa films.

DS 28.11 Thu 12:15 H8

Optical Properties and Wetting-like Behavior of Gallium Selenide Nanoflakes on Crystalline Carbon — •Raul D. Rodriguez[1], Alexander Villabona[1,2], Susanne Müller[1], Philipp Tonndorf[3], Rudolf Bratschitsch[3], Santos A. Lopez-Rivera[2], and Dietrich RT Zahn[1] — [1]Semiconductor Physics, Chemnitz University of Technology, Chemnitz, Germany — [2]Universidad de Los Andes, Laboratorio de Física Aplicada, Merida, Venezuela. — [3]Dynamics of Nanoscopic and Mesoscopic Structures, Chemnitz University of Technology, Germany

Two-dimensional (2D) materials have become the focus of research in recent years due to the remarkable physical properties observed in structures such as graphene. In this context, other 2D systems like gallium selenide and gallium sulfide have been investigated for a variety of applications from transistors to photodetectors. In this work we report on the study of the optical and the structural properties of high quality GaSe nanoflakes deposited on highly oriented pyrolitic graphite (HOPG). AFM observations show that GaSe layers adopt the morphology of the underlying carbon in a wetting-like behavior. Such strong interaction can be presumably attributed to van der Waals interaction non-screened in this system due to the high hydrophobicity of both substrates. Spatially resolved Raman and photoluminescence spectroscopies reveal a strong anisotropy on the edges and the stripe-like defects of the GaSe nanoflakes. It is found that GaSe regions with highest Raman activity and luminescence are located on crystal borders with a minor contribution from the basal crystal planes.

DS 28.12 Thu 12:30 H8

Strain analysis of CVD graphene — •Gerald V. Troppenz, Marc A. Gluba, Jörg Rappich, and Norbert H. Nickel — Helmholtz-Zentrum für Materialien und Energie GmbH

Biaxial compressive strain is induced in single layer CVD graphene grown on polycrystalline copper foil. It is generated during thermal quenching by the mismatch of thermal expansion coefficients of graphene and Cu. In situ Raman spectroscopy was used to study the phonon softening of graphene's 2D phonon mode during the transfer from Cu to thermal SiO_2. By determining the strain and stress sensitivities of the 2D phonon mode of biaxial compressed CVD graphene on Cu, we quantify the strain relaxation and the residual strain.

DS 28.13 Thu 12:45 H8

Transport properties of graphitized polymers — •Andreas Geworski, Yuri Koval, and Paul Müller — Department of Physics and Interdisciplinary Center for Molecular Materials, Universität Erlangen

We are able to convert a thin surface layer of polyimide into a graphite - like material by low-energy ion bombardment. We have found that the graphitized layer shows conductivities, which increase with the temperature of the polyimide during the ion irradiation process and which can reach more than 103 S/cm. The thickness of the graphitized layers is so low, that the films are rather transparent, which makes them interesting for carbon based optoelectronics. The optical properties were investigated in the wavelength range of 400nm-1100nm and compared to electrical measurements. The transition from insulating to semi metallic behavior already observed in the transport measurements appears in optical characterization, too. Standard interpretations like closing of an optical band gap are discussed.

DS 29: Focus Session: Organic Materials for Spintronics: From Spinterface to Devices (jointly with HL, MA, O)

Since the first report of an organic spin valve in 2004, novel devices such as spin-OLEDs (organic light emitting diodes) and spin-OFETs (organic field effect transistors) as well as sensors based on magnetic resonance were developed. This rapid development of the field of organic spintronics is driven by the large spin life time in organic molecules, combined with the large diversity and flexibility of molecular synthesis and technological processing. Despite the tremendous progress, there are still many challenges which must be tackled. On one hand, it is desirable to achieve a computer-aided design for novel molecules that can keep their properties at the interfaces with the spin-injecting electrodes. On the other hand, novel technologies for the fabrication of spin devices and the spin transport properties of various molecules are being tested. Last but not least, the spin injection at spinterfaces, i.e. at the interface between the organic molecules and the ferromagnetic electrodes, is a key factor that still needs to be understood and controlled. This topical session aims to give an overview of the latest developments in the dynamic field of organic spintronics. (Organizers: Martin Aeschlimann, Uni Kaiserslautern; Bernd Büchner, IFW Dresden; Dietrich R. T. Zahn, TU Chemnitz)

Time: Thursday 9:30–13:30 Location: H32

Invited Talk DS 29.1 Thu 9:30 H32

Organic Magnetoresistance: The effect of excitons on charge transport in organic semiconductors — •William Gillin — Queen Mary, University of London, UK

It has been known since 2003 that applying a magnetic field to an organic light emitting diode (OLED) will cause changes in both the light output (efficiency) of a device and the current through the device (organic magnetoresistance or OMR). The observation of this phenomenon has spurred a number of models to explain the observations but these can be classified in to two broad classes: excitonic and bipolaron. As the effect of the magnetic field is to apply a small perturbation to existing spin dependent processes that are affecting charge transport and recombination, the study of OMR provides an interesting new tool for understanding these processes. In this talk I will highlight the recent developments in the study of organic magnetoresistance and illustrate that the effect probably has several components which are all acting in parallel and which can have different signs and magnetic field dependencies. By developing an understanding of the different magnetic field characteristics of different processes we may open a door on to a new way of studying the interactions responsible for the fundamental operation of organic electronic devices.

Topical Talk DS 29.2 Thu 10:00 H32

Metal-phthalocyanines: Materials for molecular spintronics — •Jens Kortus[1], Rico Friedrich[1], Torsten Hahn[1], Claudia Loose[1], and Martin Knupfer[2] — [1]TU Bergakademie Freiberg, Germany — [2]IFW Dresden, Germany

Metal-phthalocyanines (MPc) are very stable and can have different spin states depending on the transition metal ion. In this contribution we will discuss electronic, (magneto)optical and transport properties of MPc in view of possible application in spintronic devices.

In particular a recently investigated layered system of MnPc and F_{16}CoPc shows charge transfer at an interface between two metal phthalocyanines, which is investigated in detail using density functional theory. These results are of importance for the application of such interfaces in organic electronic devices because charge transfer considerably affects the energy level alignment and the transport behaviour of the respective hetero-junction. Since the transfer of charge is also connected to a transfer of spin and the hybrid system has a net spin of $S = 2$, such compounds could also be termed *spin-transfer materials* with future applications in the area of spintronics [1].

[1] S. Lindner, M. Knupfer, R. Friedrich, T. Hahn, J. Kortus Phys. Rev. Lett. 109 (2012) 027601-1/5

Topical Talk DS 29.3 Thu 10:30 H32

Magneto-optical Kerr Effect Spectroscopy of Selected Phthalocyanines and Porphyrines — •Georgeta Salvan[1], Peter Robaschick[1], Frank Lungwitz[1], Michael Fronk[1], Carola Mende[1], Heinrich Lang[1], Rico Friedrich[2], Jens Kortus[2], and Dietrich R.T. Zahn[1] — [1]TU Chemnitz, 09126 Chemnitz, Germany — [2]2TU Bergakademie Freiberg, Freiberg 09596, Germany

Phthalocyanines and porphyrines find nowadays many applications from pigments to organic electronics. Nevertheless, they still have a special charm for fundamental investigations thanks to the large flexibility of their molecular structure. This work focuses on the influence of the molecular spin ground state on the room temperature magneto-optical activity of some phthalocyanines and porphyrins. The films in the typical thickness range between 30 nm and 100 nm were prepared by organic molecular beam deposition in high vacuum. Magneto-optical Kerr effect (MOKE), which is commonly used to study the magnetic properties of inorganic ferromagnetic layers or magnetic nanostructures, is measured here spectroscopically in the region of the Q and B absorption bands of phthalocyanines and porphyrines. From this the magneto-optical Voigt constant is calculated numerically and can be correlated to the electronic properties of the molecules. For instance, the hybridisation of Co3d states with the HOMO π-orbital of CoPc leads to additional features in the magneto-optical spectra compared to e.g. CuPc. The magnitude of the Voigt constant in the Q band is hardly sensitive to the molecular spin, but highly sensitive to the orientation of the molecules with respect to the substrate plane.

Topical Talk DS 29.4 Thu 11:00 H32

Molecular Quantum Spintronics — •Mario Ruben — Institut für Nanotechnologie (INT), Karlsruhe Institut für Technologie (KIT) — Institut de Physique et Chimie (IPCMS); Université de Strasbourg (UdS)

Molecules can be considered as physical Quantum Objects. Magnetic molecules consist of an atomic core of one-to-few open spin ions surrounded by a shell of organic material. At low temperature such molecular spin objects behave as simple, few-level systems.[1,2] Since quantum coherence and stable entanglement of electron spins are extremely difficult to achieve, alternative concepts propose the use of nuclear spins as quantum information carrier. Nuclear spins are extremely well isolated from environment and less prone to decoherence, and the coherent manipulation can be adapted by tailoring the molecular environment. However, although being well isolated from their surroundings, nuclear spins have to be addressed, ideally electronically since complementary with existing technologies. The delicate balance between decoupling of the magnetic molecule for stable coherence and connecting it for read out can be carried out by synthetic engineering of the molecular components. The first example of a completely electronic read out of a nuclear spin of a lanthanide ion (bearing electron and nuclear spins) embedded in a magnetic molecule TbPc2, was recently reported.[3] [1] M. Urdampilleta et.al. Nature Mater. 10, 502 (2011) [2] J. Schwöbel, et. al. Nature Comms. 2, 1953 (2012) [3] R. Vincent, et. al. Nature 488, 357 (2012)

Coffee break (15 min)

Topical Talk DS 29.5 Thu 11:45 H32

Nanomembrane based electrodes for contacting ultra-thin organic layers — •Carlos Cesar Bof Bufon[1], Celine Vervacke[2], Maria Esperança Navarro Fuente[2], Dominic J. Thurmer[2], Christian Müller[5], Michael Fronk[3], Georgeta Salvan[3], Dietrich R. T. Zahn[3], and Oliver G. Schmidt[2,4] — [1]Brazilian Nanotechnology National Laboratory, CNPEM, PO Box 619, 13083-970, Campinas, Brazil — [2]Institute for Integrative Nanosciences, IFW Dresden, Helmholtzstraße 20, 01069, Dresden, Germany — [3]Semiconductor Physics, Chemnitz University of Technology, Reichenhainerstrasse 70, 09107, Chemnitz, Germany — [4]Material Systems for Nanoelectronics, Chemnitz University of Technology, Reichenhainerstrasse 70, 09107 Chemnitz, Germany — [5]Physics Departament, UFPR, Curitiba, Brazil

One of the main challenges for accessing the electronic properties of ultrathin organic layers (UOL), and consequently their application for future devices, consists of connecting such layers to the external word. Two main problems usually arise by trying to vertically connect UOLs: i) the interdiffusion of metallic atoms into the sub-10nm molecular layers, which leads to the damaging and/or the modification of the final device behavior; ii) the presence of pin-holes across the molecular layer, which is responsible for short circuited junctions. Here we discuss the fundamentals, potentialities and limitations of using rolled up nanomembranes as top electrodes for contacting a variety of UOLs, including self-assembled monolayer's and ultra-thin organic semiconducting layers.

Topical Talk DS 29.6 Thu 12:15 H32

Spinterfaces as microscopic spin traps — •Mirko Cinchetti — Department of Physics and Research Center OPTIMAS, University of Kaiserslautern, Kaiserslautern, Germany

Interfaces between ferromagnetic materials and organic semiconductors - also known as spinterfaces - constitute an incredibly rich playground in the field of spintronics. For example, spinterfaces have the potential to be implemented as tunable spin filters, which will pave the way to a whole new class of advanced, i.e., actively controlled spintronics devices. The progress in the field of spinterface science depends thus critically on elucidating the still unexplored spin-dependent carrier dynamics at such hybrid interfaces.

We use time-resolved two-photon photoemission to optically pump and probe a hybrid electronic state forming at the prototypical spinterface between cobalt and the organometallic complex tris(8-hydroxyquinolinato)aluminium (Alq3). We generate a transient spin polarization in the hybrid interface state, and follow its behavior in four dimensions: energy, time, spin and momentum. We find that electrons are confined at the Co-Alq3 interface for times in the range of 0.5-1 ps, and that the confining potential is strongly spin dependent. Such spin-dependent trapping behavior elucidates the fundamental microscopic origin of the spin-filtering properties at spinterfaces, which is important for the design of next-generation spintronics devices based on tunable organic spin filters.

DS 29.7 Thu 12:45 H32

ESR study of the magnetic properties of the MnPc − F_{16}CoPc dimer — •Azar Aliabadi, Susi Linder, Martin Knupfer, Yulia Krupskaya, Vladislav Kataev, and Bernd Büchner — IFW Dresden, 01069 Dresden

Photoemission spectroscopy has demonstrated a charge transfer at the interface between two transition metal phtalocyanines (MnPc and F_{16}CoPc) indicating the formation of a MnPc$^{\delta+}$/F_{16}CoPc$^{\delta-}$ heterojunction [1]. In this work, the MnPc-F_{16}CoPc dimer system with charge transfer was investigated using ESR spectroscopy at different temperatures. Comparison between ESR spectra of the parent compounds (MnPc and F_{16}CoPc powders) and of the product of the reaction (MnPc/F_{16}CoPc mixed powder) has revealed characteristic features due to the formation of the MnPc − F_{16}CoPc dimer. We discuss distinct magnetic properties of the MnPc − F_{16}CoPc dimer and their possible relation to the charge transfer in the studied complex.

[1] S. Lindner, M. Knupfer, R. Friedrich, T. Hahn, and J. Kortus, *Phys. Rev. Lett.* **109**, 027601 (2012).

DS 29.8 Thu 13:00 H32

Influence of surface interaction on the properties of single-molecule-magnets — •David Klar[1], Andrea Candini[2], Bernhard Krumme[1], Loic Joly[3], Svetlana Klyatskaya[4], Jean-Paul Kappler[3], Mario Ruben[3,4], and Heiko Wende[1] — [1]Fakultät für Physik und CENIDE, Universität Duisburg-Essen — [2]Centro S3 Modena, Istituto Nanoscienze - CNR — [3]Institut de Physique et Chimie des Matériaux de Strasbourg, Université de Strasbourg — [4]Institute of Nanotechnology, Karlsruhe Institute of Technology

Due to the consecutive downsizing of devices, single-molecule-magnets as building blocks for spintronic applications are of high interest for actual research. The remanent behavior, caused by the single-ion anisotropy, of $TbPc_2$ molecules in bulk samples at less than 5 K is reported in the literature. Our goal is to investigate and to understand the influence of the surface on the properties of the $TbPc_2$ molecules deposited onto a substrate. Therefore we study submonolayer coverages of $TbPc_2$ molecules on ferromagnetic surfaces like Ni, and on a very inert surface of highly oriented pyrolytic graphite (HOPG) that should maintain the properties of isolated molecules. By XAS and XMCD we analyze the element specific magnetic and electronic properties. The low interaction with the HOPG surface hardly affects the magnetic properties of the molecules and we were able to observe a remanent magnetization, but only at very low temperatures ($T < 4$ K). On the Ni surface an indirect exchange leads to an antiferromagnetic coupling between the molecules and the surface. As a result, we obtained a remanent magnetization at higher temperatures ($T \approx 100$ K).

DS 29.9 Thu 13:15 H32

Paramagnetic organic radicals on rutile TiO2(110) single crystals — •Reza Kakavandi, Sabine-Antonia Savu, Thomas Chassé, and Maria Benedetta Casu — Institute of Physical and Theoretical Chemistry, University of Tübingen, Germany

A novel class of organic compounds, namely the nitronyl nitroxide radicals, has recently gained attention because of its magnetic property. In this work a pyrene-substituted nitronyl nitroxide radical (NitPyn) deposited on well characterized rutile TiO2(110) single crystals has been investigated by using X-ray photoemission spectroscopy (XPS) and near edge X-ray absorption fine structure spectroscopy. The mechanism of molecular adsorption on the well defined surface, the chemical environment at the interface and the electronic structure of thin films are discussed by analyzing the XPS core level signals. The persistence of the paramagnetic character of the molecules is also discussed with respect to the chemisorption on the surface. Our studies clarifies the orientation of the molecule in the thin films as a function of film thickness as well as the influence of the substrate, identifying the fine balance between molecule-molecule and molecule-substrate interactions.

DS 30: Thin Film Characterization: Structure Analysis and Composition (XRD, TEM, XPS, SIMS, RBS,...) II

Time: Thursday 14:45–17:15 Location: H32

DS 30.1 Thu 14:45 H32

CVD and ALD deposited hafnia: an XPS study — •Simone Brizzi, Massimo Tallarida, and Dieter Schmeisser — BTU Cottbus , Konrad-wachsmann allee 17 03046 Cottbus

In this work we report on Hafnium oxide deposited on silicon by means of chemical vapour deposition (CVD) and atomic layer deposition (ALD) using tetrakis-di-methyl-amino-Hf (TDMAHf) and water as precursors. We have studied the behavior of ALD and CVD at intermediate temperatures: ALD was performed outside the ALD window ($T>300$°C), whereas CVD was performed at low temperatures, approaching the ALD window ($T<400$°C). In this way we wanted to elucidate about the possibility of taking advantage of the conformality of ALD films and the high growth rate of CVD at the same time. Comparable sets of samples prepared with the two methods were measured by X-ray photoelectron spectroscopy and atomic force microscopy in order to determine differences between them: growth rate, Hf/O ratio, valence band positions and roughness are discussed and compared as a function of deposition temperature and process parameters.

DS 30.2 Thu 15:00 H32

Formation of ultrathin silica/iron-oxide epitaxial layers on Ru(0001) — •xin yu, anibal boscoboinik, bing yang, shamil Shaikhutdinov, and Hajo Freund — Fritz-Haber-Institut der Max-Planck-Gesellschaft,Berlin, Germany

Silica is one of the most abundant materials on our planet and is the key material in many modern technological applications. Thin silica films grown on metal substrates are well-suited model systems for studying structure-property relationships of silica related materials.[1] In particular, silica bilayer film weakly bound to a metal substrate can be grown on Ru(0001). This system has recently been used as a template for the preparation of aluminosilicate films.[2] In continuation of these works, here we studied preparation of Fe-doped silicate films. The experiments were carried out in an UHV chamber (base pressure < 3x10-10 mbar) equipped with LEED, AES, UPS, XPS, IRAS and STM. The film preparation includes sequential vapor deposition of Si and Fe onto an O precovered Ru(0001) substrate at ˜100 K followed by high-temperature annealing (ca. 1100 K) in ˜10-6 mbar of oxygen. The atomic structure of the resulted films was studied as a function of the Fe/Si ratio. The experimental results, substantiated by DFT calculation (performed by Sauer*s group in HU Berlin), revealed the formation of the epitaxial film consisting of a single layer of silica on top of a single layer of FeOx on Ru(0001). We believe that the prepared hetero-layered films may be interesting objects in nanotechnology. [1] S. Shaikhutdinov, H.-J. Freund, Adv. Mater., 2012. [2] J. A. Boscoboinik, et al., Angew. Chem. Int. Ed., 51 (2012) 6005

DS 30.3 Thu 15:15 H32

Composition and Chemistry of a Pd-Ni-Co thin film alloy studied by HAXPES — •Julius Kühn[1], Andreas Lippitz[1], Mihaela Gorgoi[2], Kai Nörthemann[3], Werner Moritz[3], and Wolfgang Unger[1] — [1]BAM Federal Institute of Materials Research and Testing, Berlin — [2]Helmholtz Zentrum Berlin — [3]HU Berlin

The surface near region is very important for catalytic processes. Compositional changes, e.g. segregation of alloy constituents in states before and after hydrogen sulfide exposure was investigated by non-destructive chemical HAXPES depth profiling. The HAXPES data are completed by results of AES providing data characteristic of the uppermost surface and EDX data characteristic of the bulk of the alloys.

DS 30.4 Thu 15:30 H32

Nickel Induced Crystallization of Carbon During Deposition — •Robert Wenisch, Sibylle Gemming, and Gintautas Abrasonis — Helmholtz-Zentrum Dresden-Rossendorf

A single-step process for the preparation of very thin polycrystalline carbon films on uniform nickel thin films is presented. The process temperature is significantly reduced in comparison to annealing of an amorphous carbon film without the aid of a transition metal. The degree of graphitization and the average grain size of the resulting films are examined by means of Raman-spectroscopy and transmission electron microscopy. The chemical state of the carbon atoms is analyzed by X-ray photoelectron spectroscopy. Additionally, nuclear reaction analysis is employed to confirm the temperature independence of the carbon absorption on the nickel surface. We believe that the process holds a potential for the synthesis of crystalline thin films or single layers of different 2D nanomaterials.

DS 30.5 Thu 15:45 H32

Substrate strains measured by convergent beam electron diffraction in epitaxial Ba(Fe1-xCox)2As2 thin films — •Paul Chekhonin[1], Jan Engelmann[2], Bernhard Holzapfel[2], Bernd Rellinghaus[2], Carl-Georg Oertel[1], and Werner Skrotzki[1] — [1]Institut für Strukturphysik, Technische Universität Dresden — [2]Leibniz-Institut für Festkörper- und Werkstoffforschung Dresden

Epitaxial Ba(Fe1-xCox)2As2 thin films have been produced by pulsed laser deposition on a spinel substrate with an iron buffer layer. Using the convergent beam electron diffraction technique in the transmission electron microscope, it is possible to obtain a Kossel pattern of the substrate. Strain-induced changes of the lattice parameters are derived from the captured Kossel pattern of substrate areas close to the interface with the iron buffer layer. The in-plane lattice parameters increase with respect to bulk spinel, giving evidence, that the strain in the Ba(Fe1-xCox)2As2 thin film is mainly determined by the iron buffer layer, and not by the substrate.

DS 30.6 Thu 16:00 H32

On the similarity of multiple scattering and the Moiré Effect in reciprocal space and how to make use of it in LEED — •Matthias Meissner[1], Falko Sojka[1], Marcel Grosch[1], Thomas Dienel[2], and Torsten Fritz[1] — [1]University of Jena, Institute of Solid State Physics, Max-Wien-Platz 1, 07743 Jena, Germany — [2]Empa, nanotech@surfaces, Überlandstrasse 129, CH-8600 Dübendorf, Switzerland

The effect of multiple scattering of electrons during low-energy electron diffraction (LEED) has been described decades ago. Likewise, the formation of Moiré patterns at the interface of different surface lattices is a well-known and common feature in surface physics. By definition, they are two distinct effects with different origins. However, in reciprocal space both can be treated very similarly, few assumptions provided.

It will be shown that this can be used as a powerful tool to analyze LEED patterns of systems where Moiré effects occur, e.g. Al_2O_3 on $Ni_3Al(111)$ and boron nitride on Pt(111), or in organic-inorganic hetero-epitaxy, e.g. peri-hexabenzocoronene (HBC) on graphite. Additionally, a kinematic approach to calculate spot intensities, even though imperfect to fully account for all influences on intensity, can help to understand LEED patterns, for example in the cases of few layer graphene on SiC(0001) and Al_2O_3 on $Ni_3Al(111)$.

DS 30.7 Thu 16:15 H32

Momentum-resolved Energy Loss Spectroscopy of Ultrathin Oxide Layers — •Kinyanjui Michael[1], Gerd Benner[2], Giuseppe Pavia[2], Nicolas Gauquelin[3], Gianluigi Botton[3], Hans-Ulrich Habermeier[4], Eva Benckiser[4], Bernhard Keimer[4], and Ute Kaiser[1] — [1]University of Ulm, Central Facility of Electron Microscopy, Albert-Einstein Allee 11, 89081, Ulm, Germany — [2]Carl Zeiss NTS GmbH, Oberkochen, Germany — [3]Canadian Centre For Electron Microscopy, McMaster University, 1280 Main Street West, Hamilton, Ontario, L8S 4M1, Canada — [4]Max Planck Institute for Solid State Research, Heisenbergstrasse 1, D-70579 Stuttgart, Germany, N. N.

Momentum-resolved electron-energy loss spectroscopy (MREELS) is a technique suitable for the study of momentum dependence (dispersion) of electronic excitations as well as excitations in anisotropic systems, including hidden interfaces which are hard to study with x-ray scattering. Here we report on the acquisition of MREELS spectra from ultra-thin LaNiO3-LaAlO3 layers grown on LaSrAlO4 substrate using nano-beam electron diffraction (NBED). With NBED we obtained a nearly parallel electron beam with a spot size ˜ 1.5 nm which is slightly smaller than the layer thickness of one LaNiO3 /LaAlO3 layer (layer thickness ˜ 1.7 nm). We observe features in the EELS spectra which are identified as collective electron excitations arising at the interface. This observation is supported by associated EELS spectra calculations for super-lattices. From MREELS we were also able to resolve the dispersion of the observed interfacial collective excitations.

DS 30.8 Thu 16:30 H32

Quantitative Analysis of REELS Spectra and Modeling of Optical Properties of Multilayer systems for EUV Radiation Regime — Evelyn Handick[1], •Sina Gusenleitner[1,2], Dirk Hauschild[1,3], Tina Graber[2], Dirk Ehm[2], and Friedrich Reinert[1,3] — [1]Physikalisches Institut, Experimentelle Physik VII, Universität Würzburg, 97074 Würzburg — [2]Carl Zeiss SMT GmbH, 73447 Oberkochen — [3]Karlsruhe Institut für Technologie, Gemeinschaftslabor für Nanoanalytik, 76021 Karlsruhe

Multilayer mirrors (MLM) are widely used in the extreme ultraviolet (EUV) radiation regime for various applications, but their lifetime suffers from degradation through contamination. Diverse capping layers can be used to terminate EUV MLM to protect the underlaying multilayer stack. One very promising caping material is Ru. In order to understand the time dependent influence of contaminations on these

Ru capped MLM particular heterosystems were investigated with Reflection Electron Energy Loss Spectroscopy (REELS). Analysis of the REELS spectra lead to determination of the dielectric function and various optical properties in the EUV photon energy regime which are not easily accessible by optical measurements. Furthermore, the influence of different cleaning procedures, such as Ar+ ion sputtering or atomic hydrogen cleaning, on the electronic and optical properties of the systems are monitored. Comparison of these findings with results for Ru single crystal surfaces, show the connection between the model system and the application oriented polycrystalline Ru thin-film on the heterostructure.

DS 30.9 Thu 16:45 H32

EBSD on thin FePtCu films to investigate the influence of copper content and annealing temperature on (001) texture formation and grain size — •Nathanael Jöhrmann, Herbert Schletter, Christoph Brombacher, Manfred Albrecht, and Michael Hietschold — Institut für Physik, Technische Universität Chemnitz, 09107 Chemnitz

FePt shows a very high uniaxial magnetocrystalline anisotropy in its chemical ordered $L1_0$ phase. Therefore thin FePt films are a promising candidate to raise the storage density of magnetic storage devices. For such applications it is necessary to grow films with (001) texture. The addition of copper can improve the texture formation during annealing [1-2]. To further investigate the influence of copper content on the texture formation and grain size, Electron Backscatter Diffraction (EBSD) measurements on 5-nm-thick FePtCu films with variable copper content from 0 at. % up to 21 at. % were performed. The films were prepared by magnetron sputtering of Cu/FePt bilayers at room temperature on thermally oxidized Si(100) substrates, followed by rapid thermal annealing to 600 °C for 30 s. Studies were also carried out for 15-nm-thick FePtCu films, where the annealing temperature has been varied from 500 °C to 700 °C.

Our findings suggest that copper primarily promotes nucleation of $L1_0$ (001) grains, while a higher heating temperature accelerates the crystallite growth.

[1] C. Brombacher et al., J. Appl. Phys. 112, 073912 (2012)

[2] M. Maret et al., Phys. Rev. B 86, 024204 (2012)

DS 30.10 Thu 17:00 H32

Einfache Methode zur Steigerung der Empfindlichkeit in Null-Ellipsometrie — •Marco Muth[1,2], Reiner P. Schmid[1] und Klaus Schnitzlein[2] — [1]BTU Cottbus, Institut für Physik und Chemie, LS Leichtbaukeramik, Konrad-Zuse-Straße 1, 03046 Cottbus — [2]BTU Cottbus, Institut für Verfahrenstechnik, LS Chemische Reaktionstechnik, Burger Chaussee 2, 03044 Cottbus

Die Ellipsometrie stellt eine Messmethode dar, bei der, basierend auf der Änderung des Polarisationszustandes von Licht, Brechungsindizes und Schichtdicken von Schichtsystemen, kontaktlos und schnell bis in den unteren Nanometer-Bereich untersucht werden können. In diesem Beitrag wird gezeigt, wie die geringfügige apparative Modifikation eines Null-Ellipsometers zu einer deutlich gesteigerten Empfindlichkeit der Messmethode führen kann. Beim Nachweis sehr dünner Schichten stößt das übliche Setup an seine Grenzen. Wie unsere Berechnungen und Messungen zeigen, führt eine Neujustierung des Kompensator-Azimuths, von den üblichen 45°, auf einen kleineren Wert, bei ausgewählten Schichtsystemen zu einer deutlichen Steigerung der Empfindlichkeit. Fehler werden minimiert und der Null-Findungs-Prozess optimiert. Somit ist an bestehenden Geräten eine Steigerung der Messgenauigkeit und Präzision möglich. Durch Modellrechnungen wird gezeigt, welche Schichtsysteme und Schichtdicken sich besonders eignen. Demonstriert wird die Leistungsfähigkeit der apparativen Modifikation durch Präsentation von Ergebnissen aus Messungen an den Schichtsystemen Luft/Protein/Wasser und Luft/SiO2/c-Si.

DS 31: Organic thin films II

Time: Thursday 14:45–17:00 Location: H8

DS 31.1 Thu 14:45 H8

Organic heteroepitaxy of PTCDA and SnPc on single crystalline metals — •Marco Grünewald, Kristin Wachter, Roman Forker, and Torsten Fritz — University of Jena, Institute of Solid State Physics, Max-Wien-Platz 1, 07743 Jena, Germany

Here we report on the interaction mechanisms at metal-organic and organic-organic interfaces in heterostructures of highly-ordered ultrathin layers of the dye molecules 3,4,9,10-perylene-tetracarboxylic-dianhydride (PTCDA) and tin(II)-phthalocyanine (SnPc) on Ag(111) and Au(111). The thin films were structurally characterized by Low Energy Electron Diffraction (LEED) and Scanning Tunneling Microscopy (STM) as well as optically by in situ Differential Reflectance Spectroscopy (DRS). For the first monolayer PTCDA and the first monolayer SnPc we observe significant differences between the dielectric functions extracted from the DRS depending on the substrate used indicating a rather different nature of metal-organic interaction. From the structural point of view an one monolayer SnPc film on top of Au(111) arranges as a highly ordered layer with a quadratic unit cell in a point-on-line coincidence with the reconstructed Au(111) surface. PTCDA grown on top of the first SnPc layer, however, decouples from the substrate as well as from the interlayer and shows a spectral monomer-like behavior. Structural investigations indicate an ordered growth with a line-on-line coincidence between the PTCDA and the SnPc interlayer. Additional new spectral features in the optical spectra on both substrates have been observed which can be explained by a vertical compression of the organic layer in contact with the substrate.

DS 31.2 Thu 15:00 H8

***In situ* Spectroscopic Ellipsometry Monitoring of Alq_3 and α-NPD Alkali Metal Doping** — •Francisc Haidu[1], Ovidiu D. Gordan[1], Christoph Werner[2], Maciej Neumann[2], Norbert Esser[2], and Dietrich R. T. Zahn[1] — [1]TU Chemnitz, 09126 Chemnitz, Germany — [2]ISAS Berlin, 12489 Berlin, Germany

The electron- and hole-transport organic materials Tris-(8-hydroxyquinoline)-aluminium(III) (Alq_3) and N,N'-Di-[(1-naphthyl)-N,N'-diphenyl]-(1,1'-biphenyl)-4,4'-diamine (α-NPD), respectively, were investigated in their pristine and reduced form via alkali metal (AM) doping. The two organic molecules are seen as milestones in organic light emitting diode functionality, and moreover AM doped molecules show interesting magnetic, electric, and physical properties. Extensive photoemission, inverse photoemission, vibrational spectroscopy, and theoretical studies of n-doped Alq_3 and α-NPD were performed in the last decade. The optical properties of pristine materials were previously established via spectroscopic ellipsometry (SE). This work is the first SE analysis of the doping process. *In situ* SE studies in the (0.7-5.0) eV energy range were performed by a lab-based SE and extended up to 9.5 eV by a vacuum ultraviolet ellipsometer at the synchrotron facility BESSY II, Berlin. The determined optical band gaps show evolution in agreement with filling and splitting of the lowest unoccupied molecular orbital due to AM electron donation [1, 2]. [1] M. Knupfer, H. Peisert, and T. Schwieger, Phys. Rev. B **65** (2001) 033204; [2] T. Schwieger, M. Knupfer, W. Gao, and A. Kahn, Appl. Phys. Lett **83** (2003) 500.

DS 31.3 Thu 15:15 H8

Origin of pinning-levels at molecularly modified electrodes: Mixed monolayer — •Stefanie Winkler[1,2], Johannes Frisch[2], Raphael Schlesinger[2], Martin Oehzelt[1,2], Ralph Rieger[3], Joachim Räder[3], Jürgen P. Rabe[2], Klaus Müllen[3], and Norbert Koch[1,2] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, 12489 Berlin — [2]Humboldt-Universität zu Berlin, Institut für Physik, 12489 Berlin — [3]Max Planck Institute für Polymerforschung, 55128 Mainz

Our photoemission study reveals strong work function (Φ) increases by up to 2.1 eV when strong electron acceptors comprising tetrafluoro-tetracyanoquinodimethane (F4-TCNQ) or hexaazatriphenylene-hexacarbonitrile (HATCN) are deposited on indium tin oxide (ITO) surfaces (pristine ITO Φ=4.2 eV). The evolution of the sample-Φ and the hole injection barrier upon subsequent deposition of the hole transport material N,N'-bis(1-naphthyl)-N,N'-diphenyl-1,1'-biphenyl-4,4'-diamine (α-NPD) on various submonolayer acceptor-coverages is reported for the modified ITO electrodes. We find the highest occupied molecular level of multilayer α-NPD pinned 0.5 eV below the Fermi-level, when employing the acceptor interlayers. Surprisingly pinning is achieved at a 0.4 eV (5.2 eV) higher initial Φ

than one would expect according to the ionization energy of α-NPD (IE=5.3 eV). With a simple model including a uniform electrostatic field above the first organic layer (mixture of acceptor and α-NPD) we can assign the origin of the shifted pinning-level to be caused by the pushback effect of α-NPD completing the only partly covered monolayer.

DS 31.4 Thu 15:30 H8

Molecular Tilt Angle Determination of CuPc Deposited under Different Vacuum Conditions — •Falko Seidel, Ovidiu D. Gordan, and Dietrich R. T. Zahn — Semiconductor Physics, Chemnitz University of Technology, D-09107 Chemnitz, Germany

Thin films of organic molecules are used in applications such as organic photovoltaic cells and organic field effect transistors. Nevertheless, ring structured planar molecules have a high intrinsic anisotropy due to the delocalised highest occupied molecular orbital parallel to the molecular plane. Therefore, the electrical respectively optical properties of these devices depend on the orientation of molecules within the film, which is accessible via the complex dielectric function. Variable angle spectroscopic ellipsometry (VASE) measurements of copper phthalocyanine (CuPc) films enable to quantitatively evaluate the anisotropic complex dielectric function. Considering the ratio of the out of plane optical extinction coefficient to the in plane one (substrate plane) of a uniaxial film, one can determine the average molecular tilt angle with respect to the substrate. CuPc film growth parameters such as vacuum pressure and substrate type have a strong influence on the molecular orientation. Hence, in this work in total 26 differently prepared CuPc films deposited on hydrogen passivated silicon respectively natively oxidized silicon were investigated using VASE. A critical vacuum pressure could be estimated, below which a clear influence of the substrate on the molecular orientation was visible. Moreover, the mathematical limitations are determined taking into account the optical properties of amorphous CuPc film deposited on liquid nitrogen cooled substrates.

DS 31.5 Thu 15:45 H8

Growth of p-6P thin films on graphene studied by AFM — •Markus Kratzer[1], Stefan Klima[1], Borislav Vasić[2], Radoš Gajić[2], Aleksandar Matković[2], and Uroš Ralević[2] — [1]Institute of Physics, Montanuniversitaet Leoben, Austria — [2]Institute of Physics, University of Belgrade, Serbia

Graphene is a potential candidate as transparent and flexible electrode material in organic electronics. In this study we investigated the growth morphology of the rodlike para-hexaphenyl (6P) molecule on graphene as a model system. Exfoliated graphene transferred onto a silicon oxide support was used as substrate. Sub-monolayer amounts of 6P were deposited by means of hot wall epitaxy at substrate temperatures between 280 K and 420 K. The evolving film morphologies were investigated via atomic-force microscopy. While on the SiO2 support just 6P islands consisting of upright standing molecules were found, the 6P film on the graphene evolves needle like structures which are known to be composed of flat lying molecules [1] and which also have been observed for 6P deposited onto epitaxial graphene on Ir(111) at 350 K [2]. The needle formation on graphene is favored at elevated temperatures, resulting in 6P films solely consisting of needles for deposition temperatures over 360 K.

[1] C. Teichert, G. Hlawacek, A. Andreev, H. Sitter, P. Frank, A. Winkler, N.S. Saricifci, Appl. Phys. A 82 (2006) 665. [2] F.S.Khokhar, G. Hlawacek, R. v. Gastel, H. J. W. Zandvliet, C. Teichert, B. Poelsema, Surf. Sci. 606 (2012) 475.

DS 31.6 Thu 16:00 H8

Growth and stability: The impact of fluorination of pentacene on Cu(111) — •Hendrik Glowatzki[1,2], Georg Heimel[3], Antje Vollmer[1], Swee Liang Wong[2], Han Huang[2], Wei Chen[2], Andrew T. S. Wee[2], Jürgen P. Rabe[3], and Norbert Koch[3] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH Bessy II, Albert-Einstein-Str. 15, 12489 Berlin, Germany — [2]National University of Singapore, Department of Physics, 2 Science Drive 3, 117542, Singapore — [3]Humboldt -Universität zu Berlin, Institut für Physik, Newtonstr. 15, D-12489 Berlin, Germany

In this study, the organic semiconductor pentacene (PEN) and its fully fluorinated analogue perfluoropentacene (PFP) were investigated on Cu(111) by STM, LEED, UPS and XPS. While PEN molecules at room temperature could only be imaged by STM at full monolayer coverage, PFP was found to stabilize in disordered clusters already in the sub-monolayer regime. Moreover, PFP formed only a disordered first wetting layer, whereas for PEN long-range order was already observed for closed molecular monolayers. However, highly ordered domains of PFP molecules were found for the second layer. Supported by additional STM measurements on graphite and theoretical modelling, it was concluded that the molecular planes in this layer are inclined to the surface. Therefore, careful consideration of the structural details in the transitional growth regime from molecular mono- to multilayers emerges as a key factor to achieving a deeper understanding of metal/organic interfaces relevant for organic electronic devices.

DS 31.7 Thu 16:15 H8

In-situ x-ray scattering studies of co-evaporated organic thin films: Dependence on mixing ratio — •Rupak Banerjee, Jiří Novák, Christian Frank, Alexander Gerlach, and Frank Schreiber — Institut für Angewandte Physik - Universität Tübingen, Tübingen, Germany

Organic molecular semiconductors have attracted substantial research interests due to their attractive optical, structural and electronic properties [1]. The efficiency of an organic photovoltaic (OPV) composed of organic semiconductors mainly depends on the diffusion length of the generated exciton and the charge carrier collection at the electrodes [1]. For applications in the OPV, further enhancement of efficiency can be achieved by mixing donor and acceptor organic semiconducting molecules. One of the ways of tailoring this is by changing the mixing ratio of the constituents during co-evaporation. We present insitu and real-time depth resolved grazing incidence x-ray diffraction, grazing incidence small angle scattering and x-ray reflectivity studies on the structure of mixed C60 and Diindinoperylene (DIP) films as a function of mixing ratio. We observe enhancement in the out-of-plane ordering (very smooth films up to 20 nm) upon co-evaporation of C60:DIP thin films (in different mixing ratio) which are otherwise well known to phase separate. We also observe differences in the size of the grains of the co-evaporated thin film on changing the mixing ratio.

[1] A. Hinderhofer and F. Schreiber, Chem. Phys. Chem. 13, 628 (2012).

DS 31.8 Thu 16:30 H8

Triangular dewetting of a PCDTBT-PS blend — •Paul Freyberg[1], Ioan Botiz[1,2], and Günter Reiter[1,2] — [1]Institute of Physics, University of Freiburg, Freiburg, Germany — [2]Freiburg Institute for Advanced Studies, Freiburg, Germany

Normally the dewetting of thin polymer films results in the growth of circular holes. The symmetry of this process is well understood by current theories. Interestingly, a breaking of this symmetry is found in a particular case: We observe highly anisotropic growth of holes leading to a triangular dewetting shape for the dewetting of thin polymer blend films consisting of rigid, conjugated PCDTBT* and polystyrene (PS).

By varying physical parameters like the volume fraction or by changing the substrate we can control the transition from circular to triangular dewetting. The presence of PCDTBT in thin polystyrene films leads to symmetry breaking for all dewetting temperatures in the experiments. We tentatively explain our experimental observations by an ordering of PCDTBT molecules at the contact line, leading to a breaking of the symmetry. The triangular shape is very stable, allowing triangular growth up to large scales.

*Poly[[9-(1-octylnonyl)-9H-carbazole-2,7-diyl]-2,5-thiophenediyl-2,1,3-benzo-thiadiazole-4,7-diyl-2,5-thiophenediyl]

DS 31.9 Thu 16:45 H8

Temperature dependent growth and dewetting behavior of tetraseleno-tetracene on Au(111) and Ag(111) studied by photoelectron spectroscopy — •Jens Niederhausen[1], Steffen Duhm[2,5], Christoph Bürker[3], Qian Xin[2,6], Andreas Wilke[1], Antje Vollmer[4], Frank Schreiber[3], Satoshi Kera[2], Nobuo Ueno[2], and Norbert Koch[1,4] — [1]Humboldt-Universität zu Berlin, Institut für Physik, 12489 Berlin, Germany — [2]Graduate School of Advanced Integration Science, Chiba University, Chiba 263-8522, Japan — [3]Institut für Angewandte Physik, Universität Tübingen, 72076 Tübingen, Germany — [4]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, BESSY II, 12489 Berlin, Germany — [5]Present address: FUNSOM, Soochow University, Suzhou, P. R. China — [6]Present address: School of Physics and Microelectronics, Shandong University, 5 Hongjialou, Jinan, P. R. China

The organic donor tetraseleno-tetracene (TSeT) was vacuum deposited on Au(111) and Ag(111) with the substrates (i) at room temperature and (ii) at 77 K. For these two cases we find:

(i) High resolution X-ray photoelectron spectroscopy indicates strong chemisorption of the molecules on the metal surfaces, mitigated by the diselenide groups.

(ii) Fast dewetting of TSeT multilayers is observed for samples grown at 77 K as the temperature is gradually increased. Ultraviolet photoelectron spectroscopy measurements during sample annealing reveal that the concomitant morphological changes in the TSeT film have a significant effect on its electronic structure.

DS 32: Poster Session IV: Atomic layer deposition; Organic thin films; Organic Electronics and Phototovoltaics; Organic Materials for Spintronics - from spinterface to devices; Thin film photovoltaic materials and solar cells

Time: Thursday 17:00–20:00 Location: Poster B2

DS 32.1 Thu 17:00 Poster B2

Regimes of leakage current in ALD-processed Al2O3 thin film layers — Holger Spahr, Johannes Reinker, Tim Bülow, Diana Nanova, Hans-Hermann Johannes, and •Wolfgang Kowalsky — Technische Universität Braunschweig, Institut für Hochfrequenztechnik, Schleinitzstraße 22, 38106 Braunschweig

A recently known phenomenon at thin oxide layers with thicknesses below 40 nm is the increase of their breakdown electric field, called disruptive strength, when decreasing the layer thicknesses below 10 nm. This offers the possibility to examine the current - electric field characteristics to higher electric field strengths without an early electric breakdown.

In this contribution, we report on the identification of the current regime of trap free square law and the buildup of an S shaped current - electric field characteristic curve. This observation for ALD processed Al2O3 layers has not been mentioned in literature before. Additionally a modern model of space charge limited current (SCLC) was used to fit the S shaped characteristic and extract the associated parameters, such as mobility, density of states and the energy band gap between conduction band and trap state. In this context, it can be assumed, that the Poole-Frenkel effect does not play a significant role for the current increase after the trap filled limit (TFL).

DS 32.2 Thu 17:00 Poster B2

Barrier Properties of Nanolaminates Produced by ALD — •Barbara Wegler[1,2], Oliver Schmidt[2], and Bernhard Hensel[1] — [1]MSBT, Friedrich-Alexander Universität Erlangen-Nürnberg, Germany — [2]Siemens AG, Corporate Technology, Erlangen, Germany

The water vapor transmission rate (WVTR) of the barrier layer is crucial for the lifetime of organic devices such as organic photo detectors (OPD) or organic light emission diodes (OLED). Up to now, the standard method is to glue a glass lid to the device. An alternative is to deposit nanolaminates by using atomic layer deposition (ALD) on the device. Promising results have been reported based on Al_2O_3/ZrO_2 with a WVTR of 3.2×10^{-4} g/(m^2 day).

Sputtered ZnSnOx is known to have low WVTRs. Depositing the barrier layers based on ALD nanolaminates instead of sputtering is expected to produce layers with even less defects.

The WVTR of ZnO/SnO and Al_2O_3/SnO nanolaminates has been obtained through the degradation of calcium to calcium oxide. The transparency of the resulting layers is measured by UV-Vis spectroscopy, as the transparency is an important factor for the efficiency of OPDs or OLEDs.

DS 32.3 Thu 17:00 Poster B2

Atomic Layer deposition of TiO_2 from TDMAT and H_2O: Evolution of microstructure and resulting resistance switching characteristics — •Solveig Rentrop[1], Barbara Abendroth[1], Theresa Moebus[1], Ralph Strohmeyer[1], Alexander Schmid[2], and Dirk C. Meyer[1] — [1]Institut für Experimentelle Physik, TU Bergakademie Freiberg, Leipziger Str. 23, 09599 Freiberg — [2]Institut für Angewandte Physik, TU Bergakademie Freiberg, Leipziger Str. 23, 09599 Freiberg

Atomic layer deposition (ALD) is a well-known technique used for the fabrication of thin oxide layers for high-k-dielectrics and resistive switching memory applications. Here, we present studies on the atomic layer deposition of TiO_2 from Tetrakis(dimethylamino)titan (TDMAT) and H_2O precursors in the substrate temperature range from 150 °C to 350 °C. The effects of the deposition temperature T_s and layer thickness d on the resulting anatase and rutile phase composition are investigated by grazing incidence X-ray diffraction. For T_s above 200 °C metastable anatase is always the first crystallized phase observed. At temperatures of 250 °C and higher anatase formation is always followed by the nucleation of rutile. Our results are summarized in a $T_s - d$ phase diagram. To determine the effect of the presence of crystalline phases on resistance switching performance, current-voltage characteristics are measured for Au-TiO_2-TiN capacitor structures with amorphous, partially and fully crystalline TiO_2 layers.

DS 32.4 Thu 17:00 Poster B2

Atomic layer epitaxy of Ruddlesden-Popper film structures prepared by MAD — •Felix Massel, Sebastian Hühn, Markus Jungbauer, Markus Michelmann, Camillo Ballani, and Vasily Moshnyaga — I. Physikalisches Institut, Georg-August Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen

Ruddlesden-Popper (RP) phases can be described by the general formula $A_{n-1}A'_2B_nO_{3n+1}$, where A, A', and B are cations, O is oxygen, and n is the number of the layers of octahedra in the perovskite-like stack. When aiming at high values of n, conventional solid state synthesis produces mixtures of phases with different n and the parent perovskite rather than pure phases. Submonolayer deposition precision is a way to successfully grow single phase RP films. RP films were prepared by vacuum free metalorganic aerosol deposition (MAD), which has several advantages over physical deposition methods, especially a high oxygen pressure of $p(O_2) \approx 0.2\,\mathrm{bar}$. The films were prepared by controllable pulsed spray injections of A and B type precursor solutions into the MAD chamber. By means of optical ellipsometry, a layer-by-layer - i. e. A-O/B-O_2 - deposition was monitored in situ, giving early information on the film composition. Thin films of the $Sr_{n+1}Ti_nO_{3n+1}$ RP series were prepared for $n = 1, \ldots, 4$. Further analysis of the films' structure and morphology was done by XRD and AFM. In order to achieve single phase RP samples, a fine tuning of precursor volumes, deposition temperature, deposition rate, and pulse delay time was found to be crucial for a successful synthesis. This work was supported by IFOX of the European Community's 7th Framework Programme.

DS 32.5 Thu 17:00 Poster B2

Organic molecular ion beam epitaxy of non-volatile molecules — •Gordon Rinke[1], Stephan Rauschenbach[1], and Klaus Kern[1,2] — [1]Max-Planck Institute for Solid State Research, Stuttgart, Germany — [2]Institut de Physique de la Matiere Condensee, Ecole Polytechnique Federale de Lausanne, Switzerland

Electrospray ion beam deposition (ES-IBD) was developed in our laboratory as a technique for the deposition of non-volatile molecules on well-defined surfaces in ultrahigh vacuum.[1, 2] ES-IBD is based on the creation of intact molecular ions or clusters by electrospray ionization, which are deposited on a surface as a mass selected hyperthermal beam. In contrast to evaporation, where neutral thermal particle beams are used, ES-IBD allows for the full control of the deposition process.

Here we show several examples of crystalline film growth using ES-IBD. Organic thin films are grown in layers or islands from high flux cluster beams.[3] Many other non-volatile molecules, including highly reactive species, form two-dimensional crystals on metal surfaces.

Our results show that, despite the significant differences, ES-IBD can achieve results equivalent to conventional epitaxy. The versatility and enhanced control of the deposition process shows a way towards novel coatings with unique properties.

[1] Small, 2006, 2, 540

[2] ACS Nano, 2009, 3, 2901

[3] Adv. Mater., 2012, 24, 2761-2767

DS 32.6 Thu 17:00 Poster B2

Dithiocarbamate Monolayers for Noble Metal Surface Func-

tionalization — •Tobias Schäfer[1], Philip Schulz[1,2], Christian Effertz[1], Daniel Gebauer[1], Dominik Meyer[1], Riccardo Mazzarello[3], and Matthias Wuttig[1] — [1]I. Inst. of Physics (IA), RWTH Aachen Univ. — [2]Dept. of Elect. Engineering, Princeton Univ. — [3]Inst. for Theoretical Solid State Physics, RWTH Aachen Univ.

Organic electronic devices like organic light emitting diodes, photo voltaics and thin-film transistors are well-known for their paramount technological potential. Nevertheless the need for improved electronic alignment and contact between the active organic layers and the metal electrodes remains a crucial issue. One promising approach is to modify the organic and metal interface by introducting a self-assembled monolayer (SAM) in between. In particular high work function noble metals impose the need for a dipolar interlayer to reduce the work function to enhance electron injection into organic acceptor materials.

Here, we present dithiocarbamate (DTC) monolayers efficiently lowering the work function of noble metal surfaces by up to 2 eV, as can be measured by Photoelectron Spectroscopy (PES). This distinct work function reduction is modeled and explained by density functional theory computations (DFT) in a framework of interface dipoles. The interface dipoles stem from the formation of strong bond dipoles, intrinsic molecular dipoles and the high molecular packaging density. The latter can be experimentally verified by PES. The applicability of DTC-monolayers for enhancing electronic coupling was demonstrated in OTFT devices.

DS 32.7 Thu 17:00 Poster B2

Electrical Characterization of Copper Phthalocyanine / Amorphous Silicon Hybrid Structures — •Evelyn T. Breyer, Daniel Lehmann, and Dietrich R. T. Zahn — Semiconductor Physics, TU Chemnitz, 09107 Chemnitz, Germany

Organic-inorganic hybrid junctions combine the advantageous properties of organic and inorganic layers. The electrical properties of amorphous silicon (a-Si) strongly depend on the conditions during deposition, *e.g.* substrate temperature and hydrogen flow. By surface modification of the amorphous silicon it is intended to force copper phthalocyanine molecules to adopt a "lying down" orientation on the substrate, which favours electrical conduction through the vertical stack, and is therefore desired for photovoltaic devices.

Hydrogenated amorphous silicon (a-Si:H) was sputtered onto borosilicate glass with NiCr contact fingers by DC pulsed magnetron sputtering at a constant substrate temperature of 150 °C. Thin films of CuPc (nominal thickness up to 50 nm) were deposited onto the amorphous silicon by Organic Molecular Beam Deposition (OMBD) under high vacuum conditions (3×10^{-7} mbar). Finally, silver electrodes were thermally evaporated onto the cooled sample ($T \approx -150\,^\circ$C) without breaking the vacuum. Current-voltage measurements were performed *ex situ* directly after deposition under dark and illuminated conditions (solar simulator, AM 1.5). Temperature dependent I-V curves were recorded. Two types of current transport dominate in the chosen voltage range (-2V...2V): thermionic emission and space charge limited conduction (SCLC).

DS 32.8 Thu 17:00 Poster B2

A Systematic Growth Study of Thiazolothiazole Derivatives with Varying Deposition Parameters — •Simon Siemering, Daniel Gebauer, and Matthias Wuttig — I. Physikalisches Institut (IA), RWTH Aachen University, D-52056 Aachen, Germany

Thiophene oligomers are an important class of organic semiconductors, which have considerable potential in thin film transistor (TFT) devices. Now we want to investigate their potential as an active layer in organic photovoltaic cells (OPC) and the first step is to understand the influence of different deposition parameters on thin film formation. In the framework of this study thin films of thiazolothiazole derivatives were deposited by organic molecular beam deposition (OMBD) on Indium Tin Oxide (ITO) substrates under high vacuum conditions. The influence of varying deposition rate, substrate temperature and film thickness on structure and morphology is studied with different methods. Atomic force microscopy measurements (AFM) determine the film roughness and correlation length. Film thickness and density are measured by X-ray reflectometry (XRR) while X-ray diffraction (XRD) yields the crystallinity and texture of the sample.

DS 32.9 Thu 17:00 Poster B2

Characterisation of Trap States in Transition Metal Phthalocyanine Thin Film Transistors — •Stefan Klaes, Christian Effertz, and Matthias Wuttig — I. Physikalisches Institut (IA), RWTH Aachen University, D-52056 Aachen, Germany

The family of phthalocyanines is promissing for novel organic thin film applications. Transition metal phthalocyanines exhibit very different charge carrier mobilities dependent on the transition metal even though their structural properties remain similar. The influence of the center metal atom on charge transport properties is not yet fully understood. To obtain a deeper understanding of electronic transport in organic thin film devices the charge carrier transport of several different transition metal phthalocyanines has been investigated. To do so SiO2 bottom gate/Au top contact Organic Thin Film Transistors (OTFT) with different transition metal phthalocyanines as the active layers have been produced. Their properties like charge mobility, time-domain-effects and trap depth have been examined, in particular to determine the influence of trap states. Additionally DFT based model calculations have been performed to gain a further insight into these phenomena.

DS 32.10 Thu 17:00 Poster B2

Growth Study of Organic Thin Films - Influence of Different Growth Conditions on Structure and Morphology — •Janina Felter, Daniel Gebauer, and Matthias Wuttig — I. Institute of Physics (IA), RWTH Aachen University, D-52056 Aachen, Germany

The molecule N,N'-ditridecyl-3,4,9,10-perylenetetracarboxylic diimide (PTCDI-13) is one of the few organic materials with good n-type conductivity. Hence this compound is attractive for the application in organic thin film transistors (OTFT). In order to optimize its thin film properties and to access the full potential of this molecule, the physical processes of growth and structure formation have to be investigated. In this work PTCDI-C13 films with a thickness varying from the submonolayer regime up to 60 nm have been deposited by organic molecular beam deposition (OMBD) on gold and SiO2 surfaces. The deposition rate and the substrate temperature have been varied to study the influence of different growth conditions on structure and morphology. X-ray reflectometry (XRR) has been applied in order to measure thin film thickness and roughness. The crystallinity and texture have been determined by X-ray diffractometry (XRD), while the surface morphology has been investigated by atomic force microscopy (AFM).

DS 32.11 Thu 17:00 Poster B2

Initial steps of rubicene film growth on silicon dioxide — •Boris Scherwitzl, Walter Lukesch, Günther Leising, Roland Resel, and Adolf Winkler — Institute of Solid State Physics, Graz University of Technology, Petersgasse 16, A-8010 Graz, Austria

Studies of the initial stages of organic film growth are of great relevance for the use of organics in microelectronic devices, which became of increasing importance in a variety of applications. This contribution describes the behavior of rubicene film growth on silicon dioxide with respect to sample treatments under UHV conditions. Physical vapor deposition from a Knudsen cell was used to create films with varying thickness, from sub-monolayer up to multilayer range. The exact amount of evaporated material was determined by a quartz microbalance. A number of different analytical methods were used to examine sample and surface properties, namely Auger Electron Spectroscopy (AES) for chemical analysis, Thermal Desorption Spectroscopy (TDS) to determine desorption behavior and Atomic Force Microscopy (AFM) for a subsequent ex-situ analysis of the sample surface. It could be shown that rubicene initially forms two layers of flat-lying molecules, which will stand up and form islands at and above a certain coverage. Different desorption energies suggest that the binding of the organic molecules to the substrate material is not as strong as among the molecules themselves. Substrate conditions such as purity and roughness had no observable influence. AFM studies confirmed the dewetting of the initial layers under atmospheric conditions and showed desorption and diffusion processes happening at room temperature.

DS 32.12 Thu 17:00 Poster B2

Initial growth of ultra-thin films of pentacene on mica: Influence of water and substrate morphology — •Levent Tümbek, Roman Lassnig, and Adolf Winkler — Institute of Solid State Physics, Graz University of Technology, Austria

In recent years organic electronic devices (OFETs, OLEDs) became a highly active topic in surface science due to their novel properties. A full understanding and control of the formation of organic films is a requirement for improving existing devices and further innovation. This study describes the behavior of pentacene film growth on the model substrate mica under well controlled UHV conditions. Physical vapor deposition (PVD) was the method of choice to prepare films from submonolayers up to multilayers and a quartz micro balance was applied to determine the pentacene film thickness. Argon ion sputtering was used for modifying the surface morphology. For the characterization of the film and substrate XPS, AES, TDS and ex-situ AFM was applied. It can be shown by AFM that sputtering changed the film morphology from needle-like islands, composed of lying molecules, to dendritic islands, composed of standing molecules. In the former case a wetting layer could be identified by TDS. Furthermore, it can be demonstrated that pentacene film formation depends strongly on the partial pressure of water vapor present during deposition. Regarding the adsorption kinetics, TDS revealed that the initial sticking coefficient of pentacene on mica is smaller than unity.

DS 32.13 Thu 17:00 Poster B2

Weakly forbidden transitions in manganese(II)-phthalocyanine — •Tobias Birnbaum, Claudia Loose, and Jens Kortus — Institut für theoretische Physik, Leipziger Str. 23, 09599 Freiberg

Based on known theoretical models (for example [1]) we present a comparison of selection rules for optical transitions in porphyrins and phthalocyanines. We will focus on weakly forbidden transitions in manganese(II)-phthalocyanine and compare our results with experimental data [2].

[1] M. Gouterman, J. Mol. Spec. 6, (1961), 138

[2] M. Fronk et al., PRB 79, (2009), 235305

DS 32.14 Thu 17:00 Poster B2

The influence of molecular tilt angle on the absorption spectra of pentacene:perfluoropentacene blends — •Katharina Broch, Christoph Bürker, Johannes Dieterle, Alexander Gerlach, and Frank Schreiber — Universität Tübingen, Institut für Angewandte Physik, Auf der Morgenstelle 10, 72076 Tübingen

The understanding of the optical properties of organic semiconductor blends is not only crucial for the optimization of opto-electronic devices but also of relevance for fundamental research, since it sheds light on intermolecular interactions within the films. The absorption spectra of mixed systems can be influenced by different effects, such as charge-transfer interactions within a donor-acceptor system [1,2] or structural disorder [3,4]. Using spectroscopic ellipsometry and near-edge X-ray absorption fine structure spectroscopy (NEXAFS) we investigate equimolar mixtures of perfluoropentacene (PFP) and pentacene (PEN) grown at diverse substrate temperatures. Depending on the preparation conditions, the absorption spectra exhibit significant differences. By determining the molecular tilt angles from the NEXAFS-data and by comparing our results with the structural order and the morphology [5], we discuss the effects of film structure and molecular orientation on the optical properties. [1] F. Anger et al., J.Chem.Phys., **136**, 054701 (2011); [2] K. Broch et al., Phys.Rev.B., **83**, 245307 (2011); [3] A. Aufderheide et al., Phys.Rev.Lett, **109**, 156102 (2012); [4] K. Broch et al., *in preparation*; [5] A. Hinderhofer et al., J.Chem.Phys., **134**, 104702 (2011); [6] A. Hinderhofer and F. Schreiber, Chem.Phys.Chem., **13**, 628 (2012)

DS 32.15 Thu 17:00 Poster B2

IR spectroscopic studies of p-doped thin films of organic semiconductors — •Sebastian Beck[1,2], David Gerbert[1,2], Markus Gölz[1,2], Tobias Glaser[1,2], and Annemarie Pucci[1,2] — [1]Universität Heidelberg, Kirchhoff-Institut für Physik, INF 227, 69120 Heidelberg — [2]InnovationLab GmbH, Speyerer Str. 4, 69115 Heidelberg

In this study, the underlying mechanisms and effects of doping were investigated by means of infrared spectroscopy. We examined doped and undoped thin films of organic semiconductors, such as 4,4*-Bis(N-carbazolyl)-1,1*-biphenyl (CBP), whereas different organic (e.g. 2,3,5,6-Tetrafluoro-7,7,8,8-tetracyanoquinodimethane (F4TCNQ)) and inorganic (e.g. molybdenum oxid (MoO3)) materials were used as acceptor.

The additional charge on donor and acceptor molecules in doped systems leads to specific changes in the absorption spectra compared to the spectra of undoped thin films. From the appearance of new vibrational bands, spectral shifts, and broad electronic absorptions, information about the morphological, electronical and molecular properties of the thin films was obtained, for example, on the different segregation of organic and inorganic acceptor materials and the different degree of charge transfer between donor and acceptor.

Financial support by BMBF (project MESOMERIE) is gratefully acknowledged.

DS 32.16 Thu 17:00 Poster B2

Electrical characterization of selected matrix dopant systems via U-I measurements — •Markus Gölz[1,4], Daniela Donhauser[2,4], Eric Mankel[3,4], Wolfram Jaegermann[3,4], and Wolfgang Kowalsky[1,2,4] — [1]Kirchhoff-Institut für Physik, Universität Heidelberg — [2]Technische Universität Braunschweig — [3]Technische Universität Darmstadt — [4]Innovation Lab GmbH, Heidelberg

Understanding the electrical effects of doping of organic materials is necessary to produce efficient organic devices, such as OLEDs or organic solar cells. The electrical conductance of selected matrix dopant systems is investigated via current - voltage (I-V) measurements. Typical matrices are α-NPD(NPB), CuPc and CBP. F4-TCNQ and HATNA-F6 are used as dopants. The samples are made by thermal coevaporation under UHV conditions. The electrical measurements are carried out at room temperature and atmospheric conditions.

Specifically the α-NPD: F4-TCNQ (2.7%) samples show an increase of the conductance of a factor of ten compared to the undoped matrix. Furthermore, the space-charged-limited-current region (SCLC) in the doped matrix is shifted to higher voltages. It sets in at approximately 1.5 V compared to 0.1 V in the undoped matrix.

DS 32.17 Thu 17:00 Poster B2

Interface properties of polar phthalocyanines on silver substrates — •Małgorzata Polek, Fotini Petraki, Florian Latteyer, Heiko Peisert, and Thomas Chassé — University of Tuebingen, Institute of Physical Chemistry, Auf der Morgenstelle 18, 72076 Tuebingen, Germany

Phthalocyanines (Pcs) are promising materials for various devices like light-emitting diodes, field effect transistors and solar cells. In this context, polar Pcs are of particular interest, e.g. due to their different growth properties and the variation of the chemical reactivity. Chemical reactions at interfaces could be a route for the tuning of both electronic interface properties and the molecular orientation.

We study interface properties between polar Pcs and silver using X-ray photoelectron spectroscopy (XPS), Ultraviolet photoelectron spectroscopy (UPS) as well as optical spectroscopies. We focus on VOPc, VOPcF$_{16}$, GaClPc and AlClPc. For some interfaces a clear indication for a chemical interaction was found.

DS 32.18 Thu 17:00 Poster B2

Investigation of the electronic structure of cobalt phthalocyanine films on MnO substrates by X-ray Photoemission Spectroscopy — •Mathias Glaser, Heiko Peisert, and Thomas Chassé — Instit für Physikalische und Theoretische Chemie, Universität Tübingen, Auf der Morgenstelle 18, 72076 Tübingen

Interactions at the interface between transition metal phthalocyanines (TMPc) and metal substrates affect electronic properties of adsorbed organic molecules in many cases [1,2]. Besides metals, transition metal oxide thin films are promising substrates for applications of TMPcs; studies of these interfaces however are rare. It is known that epitaxially grown ultrathin transition metal oxide films on metals show unique chemical physical properties depending e.g. on the film thickness [3,4]. In addition, charging effects in photoemission can be avoided. In this work we investigate the electronic structure of cobalt phthalocyanine on MnO ultrathin films epitaxially grown on Ag(001) using x-ray photoelectron spectroscopy.

[1] F. Petraki H. Peisert, I. Biswas, U. Aygül, F. Latteyer, A. Vollmer, T. Chassé, J. Phys. Chem. Letters 1 (2010), 3380.

[2] F. Petraki . Peisert, I. Biswas, T. Chassé, J. Phys. Chem. C 114 (2010), 17638.

[3] M. Nagel , I. Biswas, P. Nagel, E. Pellegrin, S. Schuppler, H. Peisert, T. Chassé, Phys. Rev. B 75 (2007), 195426.

[4] S. Altieri L.H. Tjeng, G.A. Sawatzky, Thin Solid Films 400 (2001), p.9.

DS 32.19 Thu 17:00 Poster B2

In-situ X-ray reflectivity of the formation of OTS-SAMs on amorphous SiO_2 and quartz — •Hans-Georg Steinrück[1], Michael Klimczak[1], Stefan Gerth[1], Andre Beerlink[2], and Andreas Magerl[1] — [1]Lehrstuhl für Kristallographie und Strukturphysik, Universität Erlangen Nürnberg , Germany — [2]Hamburger Synchrotronstrahlungslabor am Deutsches Elektronen-Synchrotron DESY, Germany

To gather further insight into the correlation between the structure of ($C_{17}H_{37}Cl_3Si$, OTS) self-assembled monolayers and the nature of the substrate [1] we compared in-situ the growth of OTS-SAMs on amorphous SiO_2 and crystalline quartz (001) via specular X-ray reflectivity. These measurements were performed at the high resolution diffraction beamline P08, DESY

As the striking difference between these two substrates we note that the dominant reflection minima remain at a constant $\mathbf{q}$ value for amorphous SiO_2 albeit with increasing amplitude over time, indicating that the molecules attach in an island growth mode (similar to the findings of Richter et al. [2]), whereas for crystalline quartz the corresponding minima shift to lower $\mathbf{q}_z$-values signaling an increasing layer thickness during the coating as expected for a random growth mode [3].

[1] Steinrueck, H. G.; Klimczak, M.; Gerth, S.; Magerl, A. submitted 2012

[2] Richter, A. G.; Yu, C. J.; Datta, A.; Kmetko, J.; Dutta, P. Physical Review E 2000, 61, 607-615.

[3] Mirji, S. A. Surface and Interface Analysis 2006, 38, 158-165.

DS 32.20 Thu 17:00 Poster B2

X-ray reflectivity study on the growth of a porphyrin monolayer — Julia Müller, •Hans-Georg Steinrück, and Andreas Magerl — Lehrstuhl für Kristallographie und Strukturphysik, Universität Erlangen Nürnberg , Germany

We investigated the growth of a metallo porphyrin ($C_{45}H_{28}CoN_4O_2$, CoP) self-assembled monolayer on amorphous SiO_2 via X-ray reflectivity. The fractional coverage of the sample was examined as a function of the reaction time in solution and was determined by multiplying the electron density with the thickness of the monolayer, which both increase with reaction time until saturation. The thickness, corresponding molecular tilt and eletron density of the fully covered substrates compare with the findings of Griffith et al. [1].

Langmuir isotherms state that the rate of surface reactions is given as: $\frac{\mathrm{d}\theta}{\mathrm{d}t} = k_a(1-\theta)C - k_d\theta$. Integration of this equation gives the time dependence of the fractional coverage. Fitting this to the experimental data yields the adsorption rate constant for CoP on amorphous SiO_2 at the given concentration of about 0.8mM.

[1] Griffith, M. J.; James, M.; Triani, G.; Wagner, P.; Wallace, G. G.; Officer, D. L. Langmuir 2011, 27, 12944-12950.

DS 32.21 Thu 17:00 Poster B2

Optical and Magneto-optical Characterisation of Thin Films of Functionalised Tetra-phenyl-porphyrines — Frank Lungwitz, Carola Mende, •Michael Fronk, Heinrich Lang, Dietrich R.T. Zahn, and Georgeta Salvan — Chemnitz University of Technology, Faculty of Natural Sciences

Metal-organic complexes are of strong interest as active materials e.g. in organic spintronic devices. Assembling these complexes as thin films on surfaces in a well defined way is an important step towards the goal of constructing such devices. In the present work we chose the group of tetra-phenyl-porphyrines (TPP) which are in terms of size just at the limit to be evaporable in vacuum in order to obtain films with very homogeneous thickness. The molecules were functionalised by short side groups such as the methoxy group and the central metal ion was varied in order to check the impact of these modifications on the dielectric and magneto-optical properties of the films prepared by organic molecular beam deposition (OMBD) onto silicon and gold substrates. The investigations utilised the techniques Variable Angle Spectroscopic Ellipsometry and Magneto-Optical Kerr Effect spectroscopy. The optical constants obtained from ellipsometry were compared to UV-VIS data taken from material in solution and the degree of uniaxial optical anisotropy and the magneto-optical data were used to estimate the molecular arrangement on the substrates. It was found that on silicon the molecular porphyrine backbone encloses a slightly smaller angle with the substrate surface than on gold.

DS 32.22 Thu 17:00 Poster B2

Controling molecular orientation of Azaacen relatives of pentacene by substrate-choice — •Michael Klues[1], Tobias Breuer[1], Julius Kögel[2], Jörg Sundermeyer[2], and Gregor Witte[1] — [1]Physics Department, Philipps Uni. Marburg, 35032 Marburg — [2]Chemistry Department, Philipps Uni. Marburg, 35032 Marburg

Nitrogen substitution of the central ring of pentacene suggests to supply a chemical more robust but almost iso-electronic molecular compounds. However, previous studies revealed for such diaza-pentacene (DAP) an entire different crystal structure than for pentacene as well as a poor charge carrier mobility. By contrast dihydrodiaza-pentacene (DHDAP) resembles the crystalline packing of pentacene and exhibits excellent charge carrier mobility although this hydrogenation is expected to break the conjugation [1]. To gain deeper insight into the electronic and structural properties of these various acenes, thin films of all compounds were studied by means of XPS, NEXAFS and XRD. Moreover, different substrates were used since this allows a control of the molecular orientation. XPS data signify an instability of DAP during the evaporation process and suggests an degradation which could be an explanation for the poor charge carrier mobility, in addition to the disadvantageous crystal structure.

[1]Qian Miao. N-heteropentacenes and n-heteropentacenequinones: From molecules to semiconductors. SYNLETT, (3):326-336, 2012

DS 32.23 Thu 17:00 Poster B2

Fabrication of Ag-TCNQ nanowires — •Markus Baranowski and Michael Huth — Physikalisches Institut, Johann Wolfgang Goethe-University, Frankfurt am Main, Germany

A method is presented which allows to grow silver-tetracyanoquinodimethan (Ag-TCNQ) nanowires by utilizing porous aluminum oxide (Al_2O_3) templates. Ag-TCNQ nanowires are interesting because of their unique electric properties. They exhibit a reproducible I-V hysteresis which shows electrical switching [1]. Promising application of the Ag-TCNQ nanowires are therefore memory devices. The Ag-TCNQ nanowires are fabricated by sputtering Ag on one side of porous Al_2O_3 templates and subsequent covering of the Ag surface with an adhesive. Afterwards a solution reaction of TCNQ solute in acetonitrile is used to obtain the Ag-TCNQ nanowires. With this technique simultaneous fabrication of nanowires with 200nm diameter and a length of up to 15μm can be achieved.
[1]:K. Xiao et al. Adv. Funct. Mater. 2008, 18, 3043-3048

DS 32.24 Thu 17:00 Poster B2

Vibrational properties of fluorinated rubrene in thin films — •Falk Anger[1], Reinhard Scholz[2], Alexander Gerlach[1], and Frank Schreiber[1] — [1]Institut für Angewandte Physik, Auf der Morgenstelle 10, 72076 Tübingen — [2]Institut für Angewandte Photophysik, TU Dresden, 01069 Dresden

One possibility of tuning the electronic properties of organic molecules is the substitution of hydrogen end groups by fluorine. Vibrational spectroscopy can be used to obtain information about the conformation of the molecules as well as intermolecular coupling in thin films. Rubrene ($C_{42}H_{28}$) has been shown to be a suitable semiconductor for applications, for which numerous experimental efforts have been made. In this study, we present FT-IR and Raman spectra of thin films of partly ($C_{42}H_{14}F_{14}$) and completely ($C_{42}F_{28}$) fluorinated rubrene. We analyse the single component-films using DFT calculations and discuss different vibrational modes. Finally, we analyse mixtures of Rubrene, $C_{42}H_{14}F_{14}$, and $C_{42}F_{28}$ to investigate the effect of the molecular environment.
[1] F. Anger *et al.*, *submitted* (2012)
[2] T. Breuer *et al.*, J. Phys. Chem. C **116**, 14491-14503 (2012)

DS 32.25 Thu 17:00 Poster B2

Energy level alignment at interfaces between low-band-gap polymers and C60 — •Milutin Ivanovic[1], Heiko Peisert[1], Ines Dumsch[2], Michael Forster[2], Ulrich Scherf[2], and Thomas Chassé[1] — [1]Institut für Physikalische und Theoretische Chemie, Universität Tübingen, Tübingen, Germany — [2]Makromolekulare Chemie und Institut für Polymertechnologie, Bergische Universität Wuppertal, Wuppertal, Germany

In electronic devices based on organic materials, the properties of interfaces are as important as the organic substances itself. Bulk heterojunctions(BHJ)play a crucial role in several devices, such as organic light emitting devices (OLEDs), organic field-effect transistors, and organic photovoltaic devices (OPVs). As example, in bulk heterojunction solar cells the interface between the donor and the acceptor material determines the ability for charge separation and the maximal reachable open circuit voltage. We study electronic properties of interfaces between low band gap (LBG) polymers (promising candidates for donor materials in OPVs) and C60 (model molecule for the acceptor material). We focus on the LBG polymers PCPDTBT, Si-PCPDTBT, PCPDTBBT and Benzoselenadiazole-based low band gap polymers. C60 films were evaporated on doctor blade casted polymer films in UHV. The interfaces were studied using X-ray photoemission spectroscopy (XPS) and Ultraviolet photoemission spectroscopy (UPS).

DS 32.26 Thu 17:00 Poster B2

Investigation of electronic and structural properties of cobalt phthalocyanine on graphene interlayers on Ni(111) — •Hilmar Adler, Johannes Uihlein, Heiko Peisert, Małgorzata Polek, Fotini Petraki, and Thomas Chassé — Institut für Physikalische und Theoretische Chemie, Auf der Morgenstelle 18, 72076 Tübingen, Germany

Transition metal phthalocyanines (TMPcs) gained increasing attention due to their tunable properties, and therefore their application in light-emitting diodes, field-effect transistors and solar cells. Most recently, the interface between TMPcs and metal substrates raised additional interest due their important role in spintronic nanodevices. Depending on the substrate TMPcs may show strong interactions at the interface.[1] The molecule-substrate interaction at the interface can be further tuned by insertion of a buffer layer. Graphene with its exciting electronic properties is an ideal candidate for such layers. Cobalt phthalocyanine as a representative of TMPcs was investigated on Ni(111) with a graphene buffer layer by scanning tunneling microscopy. The results are compared to X-ray photoelectron spectroscopy measurements and X-ray absorption spectroscopy studies.

(1) F. Petraki, H. Peisert, U. Aygül, F. Latteyer, J. Uihlein, A. Vollmer, T. Chassé, J. Phys. Chem. C 2012, 116, 11110-11116.

DS 32.27 Thu 17:00 Poster B2

The effects of oxygen exposure on copper phthalocyanine thin films — •Tomoki Sueyoshi[1,2], Masaki Ono[1], Hiroshi Tomii[3], Masakazu Nakamura[3], and Nobuo Ueno[1] — [1]Graduate School of Advanced Integration Science, Chiba University, Japan — [2]Peter Grünberg Institut (PGI-3), JARA, Forschungszentrum Jülich, Germany — [3]Graduate School of Engineering, Chiba University, Japan

The exposure of organic semiconductor thin films to gas atmospheres, such as O2, water vapor, and air, has been reported to influence their electronic properties. The gas exposure consequently results in a short lifetime and low performance of organic devices under ambient atmosphere. Such effects have been discussed from a viewpoint of electronic properties of organic layers in relation to chemical interactions between organic molecules and gas molecules. However, there is little known about the correlation between the gas exposure effects and structural properties of organic thin films.

Here, we demonstrate that the effects of O2 gas exposure depend on the molecular packing structure of organic thin films. We investigated electronic states of a copper phthalocyanine (CuPc) thin film on graphite before and after O2 exposure using ultrahigh-sensitivity ultraviolet photoelectron spectroscopy. The highest occupied molecular orbital state of CuPc with a lying-down molecular orientation was not affected by 1 atm O2 exposure while that of CuPc with a tilted-up orientation shifted toward the Fermi level after the exposure. The O2 exposure effects may originate from a weak disorder in the molecular packing structure induced by O2 diffusion into the film.

DS 32.28 Thu 17:00 Poster B2

Recombination in organic donor-acceptor bulk heterojunction solar cells — •Jędrzej Szmytkowski — Department of Chemistry, University of Florida, Gainesville, USA — Faculty of Applied Physics and Mathematics, Gdańsk University of Technology, Gdańsk, Poland

Recombination of generated charge carriers is a dominant mechanism which causes loss of photocurrent and limits the achievement of high efficiencies in organic solar cells. In this work, we present new theoretical model of bimolecular recombination in organic bulk heterojunction photovoltaic devices. Based on analysis of excitons annihilation on polarons near interface between donor and acceptor materials, we have derived analytical formula to describe the reduced Langevin recombination, which is typically observed in such molecular systems. The model explains the dependence of recombination coefficient with charge carrier concentration and also the origin of higher orders of nongeminate recombination. In addition, we discuss the light intensity dependence of polaron concentration.

DS 32.29 Thu 17:00 Poster B2

The drying process of spin coated polytriarylamine and poly(3-hexylthiophene) thin films studied by IR spectroscopy — •Michael Sendner, Jens Trollmann, and Annemarie Pucci — Kirchhoff-Institut für Physik der Universität Heidelberg

Solution processed organic semiconductor thin films are attracting increasing interest due to the possible low cost production in a roll-to-roll printing process. However the drying of such films is not well understood yet. We analyze the drying process of spin coated polytriarylamine (PTAA) and poly(3-hexylthiophene) (P3HT) films on silicon substrates in a time frame from minutes to hours after production. For this purpose we are looking at characteristic vibrational modes of the solvents, excited by mid infrared light, as well as at film morphology. Further knowledge of the drying process will offer the possibility to control important parameters of the film formation during processing. Funding by BMBF (Polytos) is gratefully acknowledged.

DS 32.30 Thu 17:00 Poster B2

Degradation processes in naphthalene diimide n–type and flexo printed polytriarylamine p–type organic field effect transistors studied by IR ellipsometry and electrical characterizations — •Jens Trollmann, Michael Sendner, and Annemarie Pucci — Kirchhoff-Institut für Physik der Universität Heidelberg

Degradation processes in organic field effect transistors is a subject not well studied yet. Especially for printed layers there is few data available. We compare variations in mid-infrared (IR) ellipsometrical spectra of evaporated naphthalene diimide thin films with changes in the electrical properties of transistors after degradation by water vapour and heat (65°C, 85%rH). Furthermore we investigate flexo printed polytriarylamine layers degraded under the same conditions. The variations of vibrational modes of atmonic bonds during degradation reveal morphological and chemical changes in organic thin films causing losses in electrical performance. Based on this information procedures to avoid serious losses can be developed. Funding by BMBF (Polytos) is gratefully acknowledged.

DS 32.31 Thu 17:00 Poster B2

Organic heterojunctions for photovoltaic applications - How does structure influence performance? — •Ingolf Segger, Stefan Klaes, Ulrike Kuck, Dominik Meyer, Christian Effertz, and Matthias Wuttig — Institute of Physics (IA), RWTH Aachen University, 52056 Aachen, Germany

Organic donor-acceptor heterojunctions are arguably the most promising system for the use as active layers in organic solar cells. Their key feature is a very efficient exciton dissociation at the interface between donor and acceptor which is crucial for device operation. Hence, one way towards high performance organic solar cells is the enlargement of the interface area, which can be achieved by simultaneous processing of donor and acceptor in order to deposit bulk heterojunctions. For certain donor-acceptor combinations significant performance improvements for bulk heterojunctions over simple bi-layer systems have already been demonstrated.

For this study we have produced small molecule bi-layers and bulk heterojunctions based on Copper Phtalocyanine as a donor and C_{60} as well as PTCDI-C_{13} as acceptor materials. The structure of the resulting films can be tuned over a wide range by employing different substrate temperatures during evaporation in ultrahigh vacuum.

Here we present our results on the influence of structural properties on absorption, charge transport and device performance which were investigated by means of x-ray diffraction, optical spectroscopy and electrical measurements.

DS 32.32 Thu 17:00 Poster B2

Tailoring Contacts in Organic Transistors by Dithiocarbamate Monolayers — •Dominik Meyer, Christian Effertz, Franziska Martin, Ingolf Segger, Daniel Gebauer, and Matthias Wuttig — Institute of Physics (IA), RWTH Aachen University, 52066 Aachen, Germany

It is well-known that the device performance of organic field-effect transistors (OFETs) strongly depends on the device geometry: Top-contact bottom-gate (TCBG) transistors usually show much better current on-to-off ratios and higher charge carrier mobilities than bottom-contact bottom-gate (BCBG) transistors. This deficiency can primarily be attributed to the difference in the electric field distribution. However, the ability to modify metal S/D-contacts with self-assembling monolayers (SAMs) is solely provided by BC OFETs. SAMs may have a direct impact on charge carrier injection barriers by changing the work function of the metal contact. We have reported previously that the work function of gold can be lowered by 2 eV with dithiocarbamate SAMs. This decrease has been attributed to the formation of an interface dipole[1]. Hence the question arises: Is it possible to improve BCBG OFETs by minimizing the charge injection barrier employing dithiocarbamate SAMs as S/D-contact modification? In this study we present the influence of dithiocarbamate SAMs on charge transport and trap state distributions in BCBG OFETs and compare them to unmodified TCBG OFETs for different n- and p-type organic semiconductors.

[1] P. Schulz et al., 2011 MRS Fall Meeting & Exhibit U13.17

DS 32.33 Thu 17:00 Poster B2

Investigation of the interface between aluminum-doped zinc oxide sputtered on copper phthalocyanine thin films. — •Cathy Jodocy, Carolin Jacobi, and Matthias Wuttig — Institute of Physics (IA), RWTH Aachen University, 52056 Aachen, Germany

Organic based electronic devices are of considerable interest because of their wide range of possible applications and commercial potential. In optoelectronic devices such as organic solar cells, organic thin film transistors and organic light emitting diodes a transparent conductive top contact can be deposited onto an organic film. These inorganic/organic interfaces are responsible for injection or collection of charge carriers. Hence an understanding of the electronic structure of the interface region is crucial to improve the performance of these devices. In this study, thin films of the transparent conductive oxide (TCO) aluminum-doped zinc oxide (ZnO:Al) are deposited onto organic semiconductor layers by a dc magnetron sputtering process. Copper phthalocyanine (CuPc) is used as the organic donor material. Due to its very rigid crystal structure, it is supposed to withstand the impact of high kinetic energy particles generated during sputter deposition of the TCO. A detailed investigation of the interface between aluminum-doped zinc oxide and copper phthalocyanine is presented. The influence of the sputter deposition of the TCO layer onto the organic thin film is characterized with x-ray photoelectron spectroscopy and x-ray diffraction measurements.

DS 32.34 Thu 17:00 Poster B2

Interface Analysis of Thermally Evaporated Thin Noble Metal Films on PTCDI-C13 — •Carolin C. Jacobi, Daniel Gebauer, Rüdiger M. Schmidt, Christina M. M. Guntermann, Cathy Jodocy, Christian Effertz, and Matthias Wuttig — I. Physikalisches Institut (IA), RWTH Aachen University, D-52056 Aachen, Germany

In recent years optoelectronic devices based on organic thin-films have gained considerable interest. They offer a wide range of possible applications and have advantageous properties such as flexibility, applicability to large areas and low production costs. The performance of devices such as organic light emitting diodes (OLED), organic field effect transistors (OFET) or organic solar cells (OSC) depends critically on the interfaces between the different layers, e.g. the organic layer and the metal electrodes. In this study, thin noble metal top contacts (Gold and Silver) have been thermally evaporated with varying film thickness and different deposition rates on N,N*-ditridecyl-3,4,9,10-perylenetetracarboxylic diimide (PTCDI-C13), which is a promising n-type material for OFETs, because it exhibits a high electron mobility. A detailed investigation of the interface between the noble metal contact and the underlying PTCDI-C13 layer is presented. We have characterized the influence of metal evaporation on the organic layer with photoelectron spectroscopy (PS) and Rutherford backscattering spectroscopy (RBS). The morphology of the metal top layer has been investigated by scanning electron microscopy (SEM).

DS 32.35 Thu 17:00 Poster B2

Influence of PCBM on the stability of the LBG Polymer PCPDTBT — •Ulf Dettinger[1], Heiko Peisert[1], Hans-Joachim Egelhaaf[2], and Thomas Chassé[1] — [1]Eberhard-Karls-University Tübingen, Institute for Physical and Theoretical Chemistry, Auf der Morgenstelle 18, D-72076 Tübingen, Germany — [2]Belectric OPV GmbH, Landgrabenstr. 94, D-90443 Nürnberg, Germany

Organic photovoltaic (OPV) incorporates an auspicious technology for the rising energy costs of the future. While aspiring for devices with higher efficiencies, the stability of the device materials is getting more and more important. It was observed, that the electron acceptor (EA) in bulk-heterojunction solar cells can affect the stability significantly [1]. We study the influence of the commonly used EA material PC[60]BM on the stability of the promising Low-Band-Gap Polymer PCPDTBT under illumination of standard Air Mass 1.5 conditions. The Photo-Degradation of the materials was monitored using UV/VIS and FTIR transmission spectroscopy. Generally PCPDTBT exhibits an enhanced stability compared to the state of the art material P3HT. Different mechanisms for the influence of PC[60]BM on the stability of both donor materials are discussed.

[1] A. Dupuis et al. Eur. Phys. J. Appl. Phys., 2011, 56, 34104

DS 32.36 Thu 17:00 Poster B2

Orientation and self organization properties of new low band-gap polymers — •Umut Aygül[1], David Batchelor[2], Ulf Dettinger[1], Florian Latteyer[1], Milutin Ivanovic[1], Heiko Peisert[1], and Thomas Chassé[1] — [1]Eberhard Karls Universität Tübingen, Institut für Physikalische und Theoretische Chemie — [2]Karlsruher Institut für Technologie, Institut für Synchrotron Strahlung

In polymer based organic solar cells so called "Low Band-Gap" (LBG) polymers with their alternating electron-deficient and electron-rich subunits are promising donor components. The orientation and the electronic properties of these polymers play an important role in device performance and therefore a detailed understanding is necessary. The orientation was investigated via angular dependent NEXAFS (Near Edge X-Ray Absorption Fine Structure) measurements of the Sulfur K-edge as for 1s absorption edges the analysis of transitions into π^* molecular orbitals enables a relatively simple and direct determination of the molecular orientation. Obviously both the chemical and geometrical structure of the polymers determines the ability for self-organization. Consequently we studied the orientation of the LBG polymers PCPDTBT, Si-PCPDTBT and PCPDTBBT. Furthermore the influence of the acceptor molecule PCBM on the self organization properties of these polymers was studied by NEXAFS measurements of donor/acceptor blend films with varying amount of PCBM. In some cases a subsequent annealing step increases the ability for self-organization significantly.

DS 32.37 Thu 17:00 Poster B2

Comparative experimental and theoretical NEXAFS-study of Acenes and Azaacenes — •Michael Klues[1], Klaus Hermann[2], and Gregor Witte[1] — [1]Physics Department, Philipps Uni. Marburg, 35032 Marburg — [2]Theory Department, Fritz Haber Institute, 14195 Berlin

NEXAFS is a powerful tool to investigate the electronic structure of molecules and can also be used to determine the molecular orientation. However, these analyses require a precise assignment of the occurring resonances, which can be provided by modern ab-initio DFT calculations implemented e.g. in the StoBe package [1]. In this study we have measured the C1s- and N1s NEXAFS signatures of various acenes (benzene and anthracene, pentacene), aza-acenes and their hydrogenated derivatives which were compared with StoBe-based calculations. By comparing spectra of acenes and aza-acenes, we carve out the influence of the higher core charge of nitrogen on the molecular electronic structure. While this effect is quite small, a distinct effect occurs upon hydrogenation of the aza-species because the conjugation of the pi-system is reduced so that the resulting signature can be described by a superposition of a dihydropyrazine and sideways attached small acenes.

[1] K. Hermann, L.G.M. Pettersson, et al. Stobe-demon version 3.1. 2011

DS 32.38 Thu 17:00 Poster B2

Domain dimensions, in-plane orientation and chemical contrast at the nanoscale: X-ray spectromicroscopy studies of organic molecules and polymers — •Anton Zykov[1], Robert Steyrleuthner[2], Marcel Schubert[2], Tayfun Mete[3], Konstantinos Fostiropoulos[3], Peter Guttmann[3], Stephan Werner[3], Katja Henzler[3], Gerd Schneider[3], Dieter Neher[2], and Stefan Kowarik[1] — [1]Inst. of Physics, HU Berlin — [2]Inst. of Physics, University of Potsdam — [3]HZB, Berlin

Transmission X-ray microscopy (TXM) at the U41-TXM beamline at BESSY, Berlin was carried out to study polymers and molecules used for different organic optoelectronic devices. We investigate the polymers P3HT and P(NDI2OD-T2), which are photoactive materials for organic solar cells, and diindenoperylene (DIP) heterostructures as applied in OFET's. The films were deposited by spin-coating and OMDB under variation of the preparation conditions, e.g. choice of solvent, blend ratio, post-annealing temperatures and film thickness. The dimensions of domains ranging from 40 to 500nm were analyzed with the TXM resolution of $\sim$30nm at the C K-edge. By measurements of the polarization dependency we obtain information about the orientation of polymer backbones and molecules in the domains, which strongly influences their optoelectronic properties. Due to the difference in the x-ray absorption energies of the used materials we got chemical contrast of blends at a nanoscale. These results will be correlated with the properties of the materials and conclusions will be drawn regarding the processes influencing the efficiency of the devices.

DS 32.39 Thu 17:00 Poster B2

Electronic structure derived from SXPS of TiO2/C60 and AZO/C60 as model electron extraction interfaces in inverted organic solars — •Philip Reckers[1], Sara Trost[2], Thomas Riedl[2], Thomas Mayer[1] und Wolfram Jaegermann[1] — [1]Technische Universität Darmstadt — [2]Bergische Universität of Wuppertal

We present first results of our study on inverted organic solar cells (IOSC) using synchrotron induced photoelectron spectroscopy (SXPS). A typical device structure is ITO/TiO2/PCBM:P3HT/MoO3/Ag. The low work-function (LWMO) transparent metal oxide conductors TiO2 or AZO act as electron extraction layer and MoO3, with its high work-function (HWMO) as hole extractor. IV-characteristics using TiO2 show photovoltaically unvafourable s-shape while AZO shows good diode characteristic. As PCBM cannot be evaporated without destruction, we investigate the model interface TiO2/C60 and compare the derived interface band diagram to AZO/C60. The LWMOs were deposited ex-situ via ALD. The acceptor C60 was evaporated stepwise onto the LWMO. Band diagrams for the pristine materials and for the hetero-junctions are derived from SXPS spectra taken at BESSY II. The used energy gaps are derived from UV-Vis absorption spectra. The CBM/LUMO offset for TiO2/C60 is 100 meV, and for AZO/C60 is 300meV with the LUMO above the conduction band maxima. Thus there is no offset at the TiO2/C60 interface that was suspected to cause the unfavourable s-shaped IV-characteristic observed in the IOSC using PCBM.

DS 32.40 Thu 17:00 Poster B2

Ultrafast Photodynamics of the Indoline Dye D149 Adsorbed to Porous ZnO in Dye-Sensitized Solar Cells — •Nadine Heming[1,2], Egmont Rohwer[1], Christoph Richter[3], Christian Litwinski[4], Derck Schlettwein[3], and Heinrich Schwoerer[1] — [1]Laser Research Institute, Stellenbosch University, South Africa — [2]Leibniz Institute for Solid State and Materials Research Dresden, Dresden University of Technology, Germany — [3]Institute for Applied Physics, Justus-Liebig-Universität, Gießen, Germany — [4]Chemistry Department, Rhodes University, South Africa

Research in the field of dye-sensitized solar cells (DSCs) has been driven by a desire to develop versatile, sustainable and affordable sources of electrical energy. We investigate photoinduced electron transfer dynamics between surface-adsorbed Indoline D149 and porous ZnO as used in working electrodes of dye-sensitized solar cells via femtosecond transient absorption spectroscopy. In the transient absorption spectra of dye D149 in solution, we found lifetimes of the excited state absorption (ESA) of 300 ± 50 ps. The absorption spectra of the dye adsorbed to ZnO shows a faster component, which is severely quenched to decay times of 150 ± 20 fs and can be assigned to the electron-transfer from the dye molecules to the semiconductor. Transient absorption spectroscopy was also conducted on the working electrode in contact with different electrolytes. The adsorption bands of the oxidized dye molecules show regeneration times in the excess of 1 ns and are shortened by the presence of electrolytes.

DS 32.41 Thu 17:00 Poster B2

Spin properties of the interface between cobalt and metal-quinolines — •Sabine Steil[1], Andrea Droghetti[2], Nicolas Grossmann[1], Stefano Sanvito[2], Mirko Cinchetti[1], and Martin Aeschlimann[1] — [1]Department of Physics and Research Center OPTIMAS, University of Kaiserslautern, 67663 Kaiserslautern, Germany — [2]School of Physics and CRANN, Trinity College Dublin, 2, Irland

In metallorganic complexes it is expected that the metal atom plays a central role in determining the molecule electronic structure and thus the magnetic properties of hybrid interfaces formed with ferromagnetic metals. This is well known in the case of metal-phthalocyanines (MPc). In fact, recent experiments [1] have demonstrated that strong changes in the spin polarization of the MPc/cobalt interface can be induced by properly choosing the central metal atom. This is a fundamental knowledge for the design of future organic spintronics devices. As aluminium quinoline (Alq_3) is a prominent molecular candidate used in spin-valve systems [2], we investigated the effect of substituting the Al atom with either gallium or indium. The electronic structure of the molecules as well as the properties of the interfaces formed with ferromagnetic cobalt were study both, experimentally, by using different photoemission spectroscopy methods and, theoretically, with density functional theory calculations. The results will be discussed focusing on the application of different quinolines in spin-valve devices.

[1] S. Lach et al. Advanced functional Materials 22, 989 (2011)

[2] V. A. Dediu et al., Nature Mater. 8, 707 (2009)

DS 32.42 Thu 17:00 Poster B2

Towards Rolled-up Spintronic Devices - Effect of Water on Permalloy and CoPc Layers — •Peter Richter[1], Maria Esperanza Navarro Fuentes[2], Frank Lungwitz[1], Michael Fronk[1], Daniel Grimm[2], Oliver G. Schmidt[2], Dietrich R.T. Zahn[1], and Georgeta Salvan[1] — [1]Semiconductor Physics, TU Chemnitz, 09126 Chemnitz, Germany — [2]Institute for Integrative Nanosciences, IFW Dresden, 01069 Dresden, Germany

Using the technique of rolled-up nanotubes, we aim to manufacture spintronic devices made from cobalt phthalocyanine molecules (CoPc) sandwiched between ferromagnetic layers. A thin CoPc layer is deposited on top of a permalloy (Py) electrode by organic molecular beam deposition. To ensure a soft and secure contact, the top electrode is formed by a nickel layer, which is the outer part of a strain engineered nanomembrane that rolls up onto the structure. The roll-up process is triggered by exposing the system to water and thus dissolving a sacrificial germanium oxide contact layer. This preliminary study determines the effect that water will have on the magnetic and optical properties of Py and CoPc. Therefore, Py and CoPc/Py layers on Si were characterized by means of spectroscopic ellipsometry, reflection anisotropy spectroscopy as well as magneto-optical Kerr-effect spectroscopy and magnetometry - once for the fresh samples and once after exposing them together with GeO_2 to water for 4 hours. The results obtained demonstrate that an oxide layer grows on Py. The CoPc layers become optically thicker, possibly due to water incorporation. The magnetic coercitivity of both layers, however, remains unchanged.

DS 32.43 Thu 17:00 Poster B2

Investigation of the influence of graphene interlayers on the interaction between cobalt phthalocyanine and Ni(111) by X-ray photoemission and absorption spectroscopies — •Johannes Uihlein[1], Heiko Peisert[1], Mathias Glaser[1], Małgorzata Polek[1], Hilmar Adler[1], Fotini Petraki[1], Ruslan Ovsyannikov[2], Maximilian Bauer[2], and Thomas Chassé[1] — [1]Institut für Physikalische und Theoretische Chemie, Auf der Morgenstelle 18, 72076 Tübingen, Germany. — [2]Helmholtz Zentrum Berlin für Materialien und Energie GmbH, Elektronenspeicherring BESSY II, Albert-Einstein-Str. 15, 12489 Berlin, Germany.

The interactions appearing at interfaces between transition metal phthalocyanines (TMPCs) and metal substrates play an important role for electron transportation processes in optoelectronic devices and spintronic nanodevices. These molecule-substrate interactions also can drastically influence the magnetic properties of the adsorbed molecules. However, these interactions might be tuned by the insertion of an interfacial buffer layer in between the metal substrate and the adsorbed molecules. With its outstanding electronic properties, graphene promises to be an excellent candidate for the tuning of interface properties. Its influence on the interactions between cobalt phthalocyanine and a Ni(111) single crystal surface has been investigated by X-ray photoemission and absorption spectroscopies.

DS 32.44 Thu 17:00 Poster B2

Properties of Phthalocyanine Hetreojunctions for the Application as Molecular Spintronic Materials — •Torsten Hahn — Institut für Theoretische Physik, TU Freiberg, Germany

Recently charge and spin transfer at an interface between two well known transition metal phthalocyanines: MnPc and F16CoPc was observed [1]. The resulting partially charged species MnPc$\delta+$ and F16CoPcδ- show different electronic properties compared to their bulk counterparts. Density Functional Theorie investigations her with experimental photoelectron spectroscopy measurements reveal that the transferred charge is substantially confined to the two transition metal centers and that a hybrid state is formed between the two types of phthalocyanines. The impact of those findings on charge and spin transport of the heterojunction coupled to different contact materials is discussed. Additional current-voltage characteristics calculated within the non-equilibrium green functions formalism (NEGF) reveal clear predictions about the spin-filter properties of this novel material.

[1] S. Lindner et. al, Phys. Rev. Lett. 109, 027601 (2012).

DS 32.45 Thu 17:00 Poster B2

Determined Molecular Orientation of Terbium Diphthalocyanine Thin Films by Ellipsometry and Magneto-optical Kerr Effect Spectroscopy — •P. Robaschik[1], M. Fronk[1], S. Klyatskaya[2], M. Ruben[2,3], D.R.T. Zahn[1], and G. Salvan[1] — [1]TU Chemnitz, 09126 Chemnitz, Germany — [2]KIT, 76344 Eggenstein-Leopoldshafen, Germany — [3]ICPMS, 67034 Strasbourg, France

The detection and control of the molecular growth mode is a key prerequisite for fabricating opto-electronic and future spintronic devices. Thin films of the single molecule magnet (SMM) terbium diphthalocyanine, which are successfully deposited by organic molecular beam deposition on silicon substrates covered with native oxide, are investigated by means of variable angle spectroscopic ellipsometry (VASE) and magneto-optical Kerr effect (MOKE) spectroscopy at room temperature. The molecular orientation was determined from the degree of uniaxial anisotropy of the optical constants. A numerical analysis of the energy dispersion of the real and imaginary part of the complex magneto-optical Kerr rotation angle in the 1.7 eV to 5.0 eV spectral range allows the magneto-optical material constant, the so-called Voigt constant, to be determined. The amplitude of the Voigt constant provides a more sensitive measure for the molecular orientation in thin films than spectroscopic ellipsometry. While VASE and MOKE are able to yield quantitative results for the molecular angle, MOKE can even resolve slight relative differences. The organic molecules in a thin film below 10 nm were found to have molecular planes close to parallel to the silicon substrate and the tilt angle increases in thicker films.

DS 32.46 Thu 17:00 Poster B2

Electro-optical charaterization of CIGS solar cells with varied absorber compositions — •Alexander Kusch, Michael Oertel, David Stoll, Udo Reislöhner, and Carsten Ronning — Institut für Festkörperphysik, Physikalisch-Astronomische Fakultät, Friedrich-Schiller-Universität Jena, Helmholtzweg 3, 07743 Jena, Germany

The results of the electro-optical characterization of sequentially processed Cu(In, Ga)Se2 solar cells are presented. The first step of the sequential absorber layer forming process is the deposition of a multilayer system containing copper, indium and gallium on top of a molybdenum back contact. Both the multi-layer system and the back contact are deposited by DC-magnetron sputtering. In the second step this metallic precursor is reactively annealed in two steps in a selenium vapour atmosphere where it is converted to an about 2 μm thick CIGSe absorber layer. Electro-optical measurements of solar cells with such prepared absorber layers show strong variations in the resulting characteristics for different precursor compositions. The efficiency of gallium free cells can vary by up to 20% as a function of the [Cu]:[In] ratios in the range of $0.75<$[Cu]:[In]<0.95. The distribution and share of gallium within the absorber was varied and the impact on solar cell performance was investigated.

DS 32.47 Thu 17:00 Poster B2

Spatially-resolved measurements of charge carrier lifetimes in CdTe solar cells — •Martin Krausse[1], Christian Kraft[1], Hannes Hempel[1], Volker Buschmann[2], Torsten Siebert[2], Christoph Heisler[1], Werner Wesch[1], and Carsten Ronning[1] — [1]Friedrich-Schiller-Universität Jena, Physikalisch-Astronomische Fakultät, Max-Wien-Platz 1, 07743 Jena, Germany — [2]PicoQuant GmbH, Rudower Chaussee 29, 12489 Berlin, Germany

The lifetime of the minority charge carriers in polycrystalline Cadmium Telluride (pc-CdTe) for solar cell applications is a crucial material parameter and has been determined by analysis of the decay curves of the luminescence signal. Both the lateral and transversal distribution of the carrier lifetime on the surface and in the bulk of pc-CdTe material as well as the respective solar cell characteristics were measured as a function of the deposition technique, the activation treatment and the incorporation of additional group-V elements. The results are compared to prior studies.

It was found, that an activation process passivates grain boundaries and increases the carrier lifetime, which is then higher at the pn-junction than at the surface. Furthermore, nitrogen and phosphorus doping of the CdTe absorber material influences the charge carrier lifetime. The results show that the spatial resolved measurement of the carrier lifetime in pc-CdTe gives an important insight to the charge carrier dynamics of the material.

DS 32.48 Thu 17:00 Poster B2

Investigation of physical properties of doped ZnTe thin films for solar cell applications — •Waqar Mahmood — Thin Films Technology Research Laboratory, COMSATS Institute of Information Technology

Zinc telluride thin films were deposited on to glass substrate using close spaced sublimation technique. The thickness of these films was optimized by deposition time. Cu & Ag doped thin films of same thickness were considered for comparative study. XRD pattern showed polycrystalline ZnTe thin films with preferred orientation (111) having cubic phase. ZnTe thin films were immersed in Ag (NO3)2 and Cu (NO3)2 solution for different times varying from 05 min to 20 min respectively. The temperature of dopant solutions were kept at 600C * 50C throughout the doping process. Post annealing of doped ZnTe thin films was done at 3500C for 1 hour under vacuum of 10-4 mbar. In XRD spectra, the crystallite size was increased after silver and copper immersion. SEM with EDX indicated the change in grain size of as-deposited and doped samples with compositional analysis of Cu and Ag in ZnTe thin films. Optical study showed the change of energy band gap in doped samples with as deposited ZnTe also %T decreases after immersion. Resistivity of as deposited ZnTe thin films was about 106 Ω-cm. which was reduced upto 68.97 Ω-cm after Cu immersion. The resistivity was reduced up to 104 Ω-cm after Ag immersion. Raman spectra showed TO and LO modes also it was used to check the crystallinity of un-doped and doped ZnTe samples.

DS 32.49 Thu 17:00 Poster B2

optical investigation of kesterite and CIGS solar cell absorber layers — •David Sperber[1], Christoph Krämmer[1], Chao Gao[1], Manuel Löw[2], Thomas Schnabel[2], Erik Ahlswede[2], Michael Powalla[2], Heinz Kalt[1], and Michael Hetterich[1] — [1]Institute of Applied Physics, Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany — [2]Zentrum für Sonnenenergie- und Wasserstoff- Forschung Baden-Württemberg (ZSW), Stuttgart, Germany

CIGS is a well-established absorber material for thin film solar cells and efficiencies above 20% have been demonstrated. Due to its abundant components kesterite $Cu_2ZnSn(S,Se)_4$ is a very promising alternative. However optical properties and the band structure of this material are still not entirely understood. We investigate kesterite solar cells and absorbers using modulation spectroscopy techniques. The results of temperature dependent electroreflectance and photoreflectance measurements to detect fundamental and higher optical transitions will be presented and discussed.

DS 32.50 Thu 17:00 Poster B2

preparation of $Cu_2ZnSn(S,Se)_4$ thin films and solar cells by chemical bath deposition — •chao gao[1], thomas schnabel[2], erik ahlswede[2], michael powalla[2,3], heinz kalt[1], and michael hetterich[1] — [1]Institute of Applied Physics, Karlsruhe Institute of Technology (KIT), 76128 Karlsruhe, Germany — [2]Zentrum für Sonnenenergie- und Wasserstoff-Forschung Baden-Württemberg (ZSW), 70565 Stuttgart, Germany — [3]Light Technology Institute (LTI), Karlsruhe Institute of Technology (KIT)

$Cu_2ZnSn(S,Se)_4$ (CZTSSe) is a promising absorber material for thin-film solar cells. It has the suitable optical band-gap for photovoltaic energy conversion, a high optical absorption coefficient, and all its constituent elements are abundant and non-toxic. Here we show a low-cost aqueous solution approach to prepare $Cu_2ZnSn(S,Se)_4$ thin films: SnS/CuS/ZnS precursor layers were prepared by chemical bath deposition firstly and then the precursor films were selenized in a graphite box under inert gas atmosphere. By optimizing the fabrication parameters, CZTSSe thin films with good quality could be obtained. The films were characterized by XRD, SEM, EDX, etc. Finally, first CZTSSe solar cells could be fabricated the properties of which will be discussed in our contribution.

DS 32.51 Thu 17:00 Poster B2

Flash Lamp Annealing of Spray Coated Silicon Nanoparticle Films — •Daniel Bülz, Falko Seidel, Iulia G. Toader, Ronny Fritzsche, Benjamin Büchter, Alexander Jakob, Roy Buschbeck, Michael Mehring, Heinrich Lang, and Dietrich R. T. Zahn — TU Chemnitz, 09126 Chemnitz, Germany

Flash lamp annealing (FLA) of spray coated silicon nanoparticles (Si NP) is considered as a low cost alternative for thin film solar cell fabrication. In this work the effect of FLA on Si NP films produced with varying number of spray cycles is investigated by Raman spectroscopy, scanning electron microscopy, and electrical characterisation. The Si NPs are dispersed in ethanol or tetrahydrofuran + di-N-methylpyrrole-silane [$H_2Si(NMP)_2$], the latter being a silicon precursor. The organosilicon acts as glue between the Si NPs in order to achieve more compact spray coated films. The suspensions are sprayed onto a preheated substrate (molybdenum sheets and hydrogen passivated doped silicon wafers). Then the samples are treated by FLA (energy: 6,37 J/cm^2; pulse time: 900 μs; flash lamp system provided by Dresden Thin Film Technology) varying the number of flashes. The whole procedure takes place in a glove box under nitrogen atmosphere to prevent oxidation. A sputtered Ni-Cr alloy reveals ohmic contact behaviour on the FLA treated spray coated Si NP films. It turns out, that adding a silicon precursor to the Si NP suspension improves the effect of FLA on spray coated films. The Si NPs are more contiguous within the films and the amount of fused Si NPs is larger than for films sprayed from pure Si NP suspensions.

DS 32.52 Thu 17:00 Poster B2

Plasma induced nitrogen incorporation in CdTe-layers for solar cell applications — •Martin Salge, Claudia Schnitter, Christoph Heisler, Christian Kraft, and Werner Wesch — Friedrich-Schiller-Universität Jena, Institut für Festkörperphysik, Helmholtzweg 3, 07743 Jena, Germany

CdTe is a promising absorber material for solar cells considering its direct band gap of 1.5 eV. CdTe solar cells feature low production costs per watt and reach efficiencies of about 17 % on a laboratory scale. The intrinsic p-type doping level of CdTe used for solar cell application is typically 10^{14} cm^{-3}. However, the efficiency can be increased further by raising the doping level by several orders of magnitude [1]. Using group-V-elements as a dopant on tellurium lattice sites is one possibility to achieve an increase in carrier concentration. Thereby, nitrogen is a promising material because in CdTe it creates doping energy levels within the band gap close to the valence band edge. In this experiment nitrogen ions were incorporated by a plasma source simultaneously to the physical vapor deposition of the CdTe-layer. Several source parameters during the absorber deposition were varied and their effects on the solar cell characteristics were studied. It was found that the solar cell characteristics and the p-type doping of CdTe absorber layers decrease significantly with increasing acceleration voltage of the N-ions. Possible reasons for that are under investigation.

[1] Sites, J. R. und J. Pan, Thin Solid Films, 515:6099, 2007

DS 32.53 Thu 17:00 Poster B2

Modulated charge separation across disordered TiO_2 / In_2S_3 hetero-junctions — •Albert Juma, Anahita Azarpira, Christian-Herbert Fischer, and Thomas Dittrich — Helmholtz-Centre-Berlin for Materials and Energy, Hahn-Meitner-Platz 1, 14109 Berlin, Germany.

Charge separation across hetero-junctions between disordered wide gap semiconductors and suitable inorganic absorbers play a decisive role for the development not only of nanocomposite solar cells. Extremely thin coatings of Cl-free and Cl-containing In_2S_3 (In_2S_3:Cl) layers were prepared by spray ion layer gas reaction (ILGAR) on nanoporous TiO_2 (np-TiO_2). Charge separation in FTO/np-TiO_2/In_2S_3:Cl, FTO/In_2S_3:Cl, FTO/np-TiO_2 / In_2S_3 and FTO/In_2S_3 systems has been investigated by modulated surface photovoltage spectroscopy (SPV). The exponential defect tails below the band gap of In_2S_3 were reduced for In_2S_3:Cl. The analysis of the SPV spectra allowed to distinguish different mechanisms of charge separation and to deduce the conduction band offsets (about 0.3 eV and 0.05 eV for np-TiO_2/In_2S_3:Cl and np-TiO_2/In_2S_3, respectively).

DS 32.54 Thu 17:00 Poster B2

Wire-based dye-sensitized solar cells using electrodeposited zinc oxide on passivated metals — •Tim Helbig, Melanie Rudolph, and Derck Schlettwein — Justus-Liebig-University Giessen, Institute of Applied Physics, Heinrich-Buff-Ring 16, D-35392 Giessen, Germany

Metal substrates provide good properties as electrode material in dye-sensitized solar cells (DSSC) such as good processability, high conductivity and mechanical flexibility. In order to be used in DSSC the metal has to be inert against the iodine-containing electrolyte used in DSSC. Passivated metals such as tungsten, stainless steel or aluminum are covered with a natural oxide layer providing protection against corrosion and are therefore of interest as electrode materials. Zinc oxide thin films were prepared as porous semiconductor on tungsten or aluminum wires by electrochemical deposition. The indoline dye D149 was adsorbed to the surface of the porous zinc oxide as a sensitizer. The films were studied as a photo anode of a DSSC.

DS 32.55 Thu 17:00 Poster B2

Laser processing for CIGS thin-film solar cells — •Xi Wang[1,2], Dorena Fleischer[2], Pierre Lorenz[2], Martin Ehrhardt[2], Xiaowu Ni[1], and Klaus Zimmer[2] — [1]Nanjing University of Science & Technology, Xiaolingwei 200, 210094 Nanjing, China — [2]Leibniz-Institut für Oberflächenmodifizierung e. V., Permoserstraße 15, 04318 Leipzig, Germany

The Cu(InGa)Se2 (CIGS) thin-film solar cell attracts increasing attention because of its low cost, flexible character and high efficiency. Laser is an effective tool in performing the monolithic integrated interconnection and external integrated interconnection for the module fabrication. CIGS thin-film solar cells were scribed with picosecond laser with a pulse length of 10 ps and a wavelength of 1064 nm. The material modification and the electrical properties were influenced by the laser parameters such as fluence, frequency, and scanning speed. In the present study, the interaction mechanisms of CIGS thin-film solar cell material with picosecond laser beam were investigated. The laser-induced material removal and the material morphology of the laser-scribed areas were analyzed by scanning electron microscopy (SEM) and energy-dispersive X-ray spectroscopy (EDX). The electrical current voltage (I-V) curves with the open circuit voltage and parallel resistance were measured with an in situ measurement. Goal of the examination was the improvement of the generation of scribes in the CIGS material under attention to electrical properties in combination with surface characteristics for optimal preparation of further steps of production.

DS 32.56 Thu 17:00 Poster B2

Influence of surface treatments on the charge recombination characteristics in porous ZnO for dye-sensitized solar cells — •Christoph Richter, Max Beu, and Derck Schlettwein — Institute of Applied Physics, Justus Liebig University of Giessen, Heinrich Buff-Ring 16, 35392 Giessen, Germany.

ZnO films to be used in dye-sensitized solar cells (DSC) can be grown by electrochemical deposition of a porous $ZnO/EosinY$ hybrid material from an aqueous solution of $ZnCl_2$. In a subsequent step the $EosinY$ has to be desorbed to provide a porous network of ZnO for the adsorption of a sensitizer. The step of $EosinY$ desorption is performed in an aqueous solution of 10.5 pH KOH. This treatment can alter the surface of ZnO which typically leads to changes in the charge transfer characteristics (mainly recombination) at the semiconductor/electrolyte interface in the assembled DSC. In this work different methods of $EosinY$ desorption and different post-treatment steps of the surface are studied. The consequences of the different treatment steps on the charge transfer from porous ZnO to an iodine-containing electrolyte are studied by IV-curves and electrochemical impedance spectroscopy. Appropriate strategies to compensate surface changes introduced by the desorption step of $EosinY$ are presented.

DS 32.57 Thu 17:00 Poster B2

Thin magnesium silicide semiconducting films for photovoltaics — •Carina Ehrig[1,2], Ralf Krause[1], Günter Schmid[1], and Christoph Brabec[2] — [1]Siemens AG, CT RTC MAT MPV-DE, Erlangen — [2]Lehrstuhl für Werkstoffe der Elektronik- und Energietechnik, FAU Erlangen-Nürnberg, Erlangen

The semiconducting magnesium silicide (Mg_2Si) is a promising candidate for a low-cost and efficient absorber layer for solar cells. Its main application so far is as a high-performance thermoelectric material due to its high figure of merit. Little is known, however, about its applicability as a photoactive material. The metal-rich semiconducting Mg_2Si is the only stable phase in the Mg–Si system. It has a narrow indirect band gap of 0.78 eV. Its absorption coefficient of $\alpha = 3.5 \times 10^5$ cm^{-1} at 2.5 eV is about 40 times higher than that of c-Si, which makes it an interesting material for producing thin solar cells.

In the present work, Mg_2Si thin films were produced by thermal evaporation of Mg on Si substrates and subsequent annealing. This results in the formation of flat and homogeneous Mg_2Si layers, which can be adjusted in thickness by varying the annealing temperature and time as well as the amount of Mg deposited. The Mg_2Si films are characterized in terms of morphological, electrical and optical properties. Furthermore, measurements on the photoactivity of these layers will be discussed as well as several ideas for the usage of this material in solar cell devices. For example, the formation of a pn-junction consisting of a p-type silicon wafer and an n-type Mg_2Si thin layer as well as other solar cell designs are proposed.

DS 32.58 Thu 17:00 Poster B2

Electrical and structural characterization of CdTe thin film solar cells with In_2S_3 buffer layer — •Felix Lind[1], Johanna Krammer[2], Christoph Heisler[1], Christian Kraft[1], Christian-Herbert Fischer[2], and Werner Wesch[1] — [1]Friedrich-Schiller-Universität Jena, Institut für Festkörperphysik, Helmholtzweg 3, 07743 Jena — [2]Helmholtz-Zentrum Berlin für Materialien und Energie, Hahn-Meitner-Platz 1, 14109 Berlin

As an alternative to the commonly used toxic CdS, in this work In_2S_3 is used as n-type buffer layer in CdTe thin film solar cells. In contrast to CdS, In_2S_3 can be deposited in a non-vacuum process at low temperatures without producing toxic waste. The In_2S_3 buffer layers with varied chlorine concentrations and thicknesses were fabricated with the "ion layer gas reaction" (ILGAR) process. Subsequently the CdTe layers were deposited by the physical vapour deposition (PVD) method. The electrical properties of the complete solar cells were investigated by means of current-voltage measurements (I-V) and external quantum efficiency (EQE). The results show that the conversion efficiencies and quantum efficiencies are significantly lower for the CdTe thin film solar cells with In_2S_3 buffer layer compared to solar cells with CdS buffer layer. Scanning transmission electron microscopy (STEM) was used to investigate the structural properties. It was found that the post deposition $CdCl_2$-treatment leads to a non-uniform and lower thickness of the In_2S_3 layer. Altogether CdTe solar cells with In_2S_3 buffer layer are producible in principle at the used process parameters, but show no improvement compared to CdS buffer layer.

DS 32.59 Thu 17:00 Poster B2

Composition-dependent atomic-scale structure of $Cu(In,Ga)S_2$ — •Stefanie Eckner[1], Helena Kämmer[1], Tobias Steinbach[1], Martin Gnauck[1], Andreas Johannes[1], Christiane Stephan[2], Susan Schorr[2], and Claudia Sarah Schnohr[1] — [1]Institut für Festkörperphysik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany — [2]Helmholtz-Zentrum Berlin für Materialien und Energie, Hahn-Meitner-Platz 1, 14109 Berlin, Germany

In order to exploit the full potential of $Cu(In,Ga)S_2$-based thin film solar cells, a deeper understanding of the composition-dependent atomic-scale structure along with its influence on electrical properties such as the band gap is necessary. In this study, element-specific first nearest neighbour distances of $Cu(In,Ga)S_2$ were determined as a function of the In/(In+Ga) ratio using extended X-ray absorption fine structure spectroscopy. All three bond lengths, namely Cu-S, Ga-S and In-S, are found to differ from each other and to remain nearly constant over the whole compositional range of $0 \leq In/(In+Ga) \leq 1$ despite the significant change of the lattice constants. Structural parameters have also been simulated with a valence force field model for all possible first nearest neighbour configurations surrounding the S anions. Excellent agreement between the calculated average bond lengths and the experimental values is obtained for a non-random distribution of In and Ga atoms that favours a mixed Cu-In-Ga configuration over the pure Cu-In or Cu-Ga first nearest neighbour shells.

DS 32.60 Thu 17:00 Poster B2

Photoluminescence study of polycrystalline silicon thin films prepared by liquid and solid phase crystallization — •Steffi Schönau, Jörg Rappich, Moshe Weizman, Daniel Amkreutz, and Bernd Rech — Kekuléstr. 5, 12489 Berlin

Polycrystalline silicon thin films were prepared by depositing amorphous or microcrystalline silicon layers onto glass substrates and subsequent crystallization via solid or liquid phase crystallization approaches. Differences in layer morphology and quality were characterized using low temperature photoluminescence (PL) spectroscopy and electron backscatter diffraction spectroscopy. The analysis of spectrally and spatially resolved photoluminescence from poly-Si thin films was shown to be an useful tool for a fast characterization of the sample recombination behavior of light induced charge carriers.

DS 32.61 Thu 17:00 Poster B2

A study of compensation in CZTSSe absorber layers by Photoluminescence spectroscopy and Capacitance-Voltage profiling — •Steffen Kretzschmar, Sergej Levcenko, Justus Just, and Thomas Unold — Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Institut für Technologie, Hahn-Meitner-Platz 1, D-14109 Berlin

With the demonstration of a conversion efficiency of 11.1% the potential of $Cu_2ZnSn(S,Se)_4$ (CZTSSe) as an alternative absorber material for thin film photovoltaics has been confirmed. Nevertheless only little knowledge exists on the electronic properties in the bandgap. Especially a thorough understanding of beneficial electronic properties and their dependence on the chemical composition of the material is needed to improve the CZTS solar cell performance further.
Here a study by Photoluminescence (PL) spectroscopy of absorber layers in a wide range of composition is presented. Excitation and temperature dependent PL-measurements are carried out and are related to the findings from Capacitance-Voltage (CV) profiling on solar cells made of absorber layers from the same growth process. The results exhibit a beneficial influence of compensation by donors on the conversion efficiency of CZTSSe solar cells.

DS 32.62 Thu 17:00 Poster B2

Development of a Laser based Zinc oxide treatment for the systematic variation of electro-optical properties — •Erik Schumann[1,2], Stefan Haas[2], and Jürgen Hüpkes[2] — [1]Helmholtz-Zentrum Dresden-Rossendorf, D-01314 Dresden, Germany — [2]IEK5 - Photovoltaik, Forschungszentrum Juelich GmbH, D-52425 Juelich, Germany

Zinc oxide is a widely used transparent conductive oxide (TCO), e.g. as front contact for thin film solar cells. Though already having a low absorption in the visible spectral range and a good conductivity, magnetron sputtered zinc oxide can be improved to increase the performance of thin film solar cells [1,2]. A laser treatment was developed to improve the electrical and optical properties of this material. The influence of the different process parameters were investigated. In addition, the effect of the ambient atmosphere, i.e. oxygen and nitrogen, were analysed. Different schemes to prevent exposure of zinc oxide to ambient atmosphere during laser treatment will be presented. This work is part of the LIST project (BMU: 0325299). [1] M. Berginski, PhD thesis, RWTH Aachen, FZ Juelich (2007) [2] M. Wimmer et. al., Thin Solid Films 520, 4203 (2012)

DS 33: Plenary Talk - Caroline Ross

Time: Friday 8:30–9:15 Location: H1

Plenary Talk DS 33.1 Fri 8:30 H1

Templated Self-assembly of Block Copolymer Films — •Caroline Ross — Massachusetts Institute of Technology, Cambridge, MA, USA

The microphase separation of block copolymer films produces periodic nanoscale patterns with feature sizes of a few nm and above, and has been proposed as a method for extending microelectronic fabrication beyond the limits of optical lithography. To control the long range order of the microphase separation, and to produce patterns with designed aperiodic features, templating strategies based on substrate topography have been developed in combination with modeling using self consistent field theory. The structures formed by self-assembly are governed by commensurability between the template and the equilibrium period of the block copolymer. The templating of complex patterns such as 3D cross-point structures from bilayer films of a diblock copolymer, and arrays of rings, square-symmetry posts and Archimedean tiling patterns from linear or star triblock terpolymers will be described. Pattern transfer and applications to nanoscale device fabrication will be discussed.

DS 34: Resistive Switching (jointly with DF, KR, HL)

Time: Friday 9:30–12:45 Location: H32

DS 34.1 Fri 9:30 H32

***Ab initio* study of defects in SrTiO$_3$ bulk and (100) surfaces** — •Ali Al-Zubi, Gustav Bihlmayer, and Stefan Blügel — Peter Grünberg Institut (PGI) & Institute for Advanced Simulation (IAS), Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

Oxygen vacancies are believed to play a major role in the conduction mechanisms that enable resistive switching in oxide materials. Employing density functional theory (DFT) and the DFT+U model,we use the full-potential linearized augmented plane wave method as implemented in the `FLEUR` code to study the formation of point defects in the perovskite SrTiO$_3$ with varying coordination. We calculated the formation energy of an O-vacancy in both bulk supercells and (100) surface including different, c(2×2) and p(2×2), in-plane unit cells and different terminations. After performing full relaxation, we found that the bulk and SrO-terminated surface have a nonmagnetic, while TiO$_2$-terminated surface has a ferromagnetic solution. Using the c(2×2) unit cell, the vacancy formation energy was smaller for the bulk than for the SrO- and even TiO$_2$-terminated surface. On the other hand, the p(2×2) unit cell shows that TiO$_2$-terminated surface has the lowest formation energy, more than 1 eV lower than the bulk value. Similar comparisons will be presented when including the the DFT+U model that is used to correct the bulk bandgap and improve the localization of the defect states.

We gratefully acknowledge financial support of the DFG, SFB 917 Nanoswitches–A4 project.

DS 34.2 Fri 9:45 H32

Resistive switching properties in ion beam modified SrTiO$_3$ — •Jura Rensberg, Benjamin Roessler, Christian Katzer, Frank Schmidl, and Carsten Ronning — Institut für Festkörperphysik, Friedrich-Schiller-Universität Jena, Germany

Resistive switching phenomena, which are for instance observed in perovskite-type transition metal oxides, attract intensive attention for their potential application in future nonvolatile memory. Strontium titanate (SrTiO$_3$) exhibits bipolar resistive switching between a high- and a low-resistance state when applying an appropriate electric field. It is often proposed that the underlying mechanism for bipolar resistive switching in SrTiO$_3$ originates from oxygen-vacancy migration along filaments based on extended defects such as dislocations or grain boundaries.

Here we report on well-defined damage formation due to ion irradiation which allows a better control of the lateral and vertical defect arrangements and concentrations. Therefore, we deposited 100 nm single crystalline SrTiO$_3$ thin films with low intrinsic defect concentration on niobium doped SrTiO$_3$ substrates by pulsed laser deposition and implanted these samples with swift heavy gold ions. After irradiation the films were characterized using transmission electron microscopy and Rutherford backscattering spectrometry. Under ion irradiation, the as-deposited crystalline films undergo amorphisation due to the formation and overlap of amorphous tracks. The electrical properties of SrTiO$_3$, i.e. the resistive switching properties are discussed in terms of damage concentration.

DS 34.3 Fri 10:00 H32

Cation defect engineering in SrTiO3 thin films by PLD with Verification and implication on memristive properties — Sebastian Wicklein[1], •Chencheng Xu[1], Alessia Sambri[2], Salvatore Amoruso[2], David Keeble[3], Annemarie Köhl[1], Werner Egger[4], and Regina Dittmann[1] — [1]Peter Grünberg Institut 7, Forschungszentrum Jülich GmbH, Germany — [2]Università degli Studi di Napoli Federico II, Dipartimento di Scienze Fisiche & CNR-SPIN, I-80126 Napoli, Italy — [3]University of Dundee, School of Engineering, Physics and Mathematics, Dundee DD1 4HN, Scotland — [4]University Bundeswehr, D-85577 Munich, Germany

The origin of the c-axis expansion in homoepitaxial STO thin films is investigated by positron annihilation lifetime spectroscopy (PALS): Low laser fluence results in Ti vacancy rich sample while high laser fluence for the Sr vacancy rich sample.

XPS measurement on the ablated spot on the targets shows that increased laser fluence ablates more Ti. The ToF (Time of Flight) data from OES (optical emission spectrometry) indicate a preferred scattering of Ti because of background gas. The two effects together lead to tunable stoichiometry of the film.

In the MIM (metal insulator metal) structure Sr-rich films exhibit the most stable switching behavior and highest on/off ratio, while in the LC AFM (local conducting atomic force microscopy) switching the on/off ratio of Ti is the higest.

DS 34.4 Fri 10:15 H32

Resistive Switching in thermally oxidized Titanium — •Daniel Blaschke[1], Ilona Skorupa[1], Bernd Scheumann[1], Andrea Scholz[1], Peter Zahn[1], Sibylle Gemming[1], Kay Potzger[1], Agnieszka Bogusz[2], and Heidemarie Schmidt[2] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Institute of Ion Beam Physics and Materials Research, P.O. Box 510119, 01314 Dresden - Germany — [2]Dept. Electr. Eng. & Inf. Techn., TU Chemnitz, 09107 Chemnitz

In recent years the resistive switching of binary transition metal oxides like NiO, Nb2O5 and TiO2 has attracted considerable attention for application in nonvolatile memory storage systems.

For our investigations we used a thin rutile TiO2 film, which was prepared by the thermal oxidation of a 100nm thick e-beam evaporated Ti film. The oxidation temperatures were varied from 500°C to 800°C at an oxygen partial pressure of 1 atmosphere. We will present the dependence of the crystal structure and the switching behavior on the oxidation temperature as well as an interesting feature on the time-dependent evolution of the resistance during the Reset process.

The project is funded by the Initiative and Networking Fund of the Helmholtz Association (VH-VI-422).

DS 34.5 Fri 10:30 H32

Non-volatile resistive switching in multiferroic YMnO3 thin films — •Agnieszka Bogusz[1,2], Ilona Skorupa[1], Andrea Scholz[1], Oliver G. Schmidt[2,3], and Heidemarie Schmidt[2] — [1]Institute of Ion Beam Physics and Materials Research, Helmholz-Zentrum Dresden-Rossendorf, 01314 Dresden, Germany — [2]Faculty of Electrical Engineering and Information technology, Chemnitz University of Technology, 09107 Chemnitz, Germany — [3]Institute for Integrative Nanosciences, IFW-Dresden, 01069 Dresden, Germany

Intensive research on multiferroic materials [1] is driven by the possibility of creating novel, miniaturized tunable multifunctional devices [2]. This work investigates resistive switching behavior of YMnO3 thin films, which can be utilized in new generation memory devices. Series of YMnO3 films were grown by pulsed laser deposition on Si substrates with Pt bottom electrode at temperatures varying between 500°C and 850°C. Characterization of as-grown samples by X-ray diffraction and scanning electron microscopy was followed by determination of electrical properties of films in metal-insulator-metal (MIM) configuration. Results showed that the YMnO3 films grown at 800°C exhibit the best resistive switching properties with high resistance ratio (>10000) of high over low resistance state. Switching mechanism is ascribed to the structural transitions within the film upon applied current.

[1] A. Bogusz et al., Defect Diffus. Forum 323-325, 115 (2012)

[2] Y. Shuai, H. Schmidt et al., J. Appl. Phys. 109, 124117 (2011); J. Appl. Phys. 111, 07D906 (2012)

DS 34.6 Fri 10:45 H32

Practical guide for validated memristance measurements — •Nan Du[1,2], Yao Shuai[3], Wenbo Luo[3], Christian Mayr[4], Rene Schüffny[4], Oliver G. Schmidt[1,2], and Heidemarie Schmidt[1] — [1]TU Chemnitz, Faculty of Electrical Engineering and Information Technology, 09107 Chemnitz, Germany — [2]Institute for Integrative Nanosciences, IFW Dresden, Helmholtzstraße 20, 01069 Dresden, Germany — [3]Helmholtz Research Center Dresden-Rossendorf, 01328 Dresden, Germany — [4]TU Dresden, Department of Electrical Engineering and Information Technology, 01062 Dresden, Germany

L.O. Chua predicted rather simple charge-flux curves for active and passive memristors and presented active memristor circuit realizations already in the 70s. However, despite the fact that memristors give rise to complicated hysteretic current-voltage curves, memristors are traced in current-voltage curves. Here we give a practical guide how to use normalized charge-flux curves for the prediction of current-voltage characteristics of memristors with stable electrical characteristics in dependence on the shape and amplitude of the input voltage or input current signals. In the case of memristive BiFeO3 thin film capacitor structures [1] the normalized charge-flux curves superimpose for different numbers of measurement points and a different measurement time per measurement point. Such normalized charge-flux curve can be used for the prediction of current-voltage characteristics of plastic synapses in neuromorphic systems [2]. [1] Y. Shuai et al., J. of Appl. Phys. 109, 124117-124117-4 (2011). [2] C. Mayr et al., NIPS 2012, in press.

Coffee break (15 min)

DS 34.7 Fri 11:15 H32

Creating an Oxygen Gradient in Nb_2O_5 by Argon Irradiation for Resistive Switching Memory

— •Helge Wylezich[1], Hannes Mähne[1], Daniel Blaschke[2], Stefan Slesazeck[1], and Thomas Mikolijack[1] — [1]NamLab gGmbH, Nöthnitzer Str. 64, D-01187 Dresden — [2]Helmholtz-Zentrum Dresden-Rossendorf, D-01314 Dresden

It is common knowledge that an oxygen gradient is mandatory for bipolar resistive switching [1]. We confirmed this by investigations of thin films with Nb_2O_5 as switching layer. Samples with two inert Pt electrodes are nearly symmetric and do not show bipolar resistive switching behavior. Replacing one Pt electrode with a reactive one – for example Al or Nb – results in an unsymmetrical device. These samples could be switched reproducible. It is also possible to create an oxygen gradient by depositing a stack of two different niobium oxide layers. While the first layer consists of stoichiometric Nb_2O_5 the second layer is sputtered substoichiometric [2].

A new approach is to get an oxygen gradient by irradiating the oxide layer with argon. Two effects appear: The argon sputters the surface of the Nb_2O_5 layer and so the oxide thickness decreases. Because the Nb-atoms are heavier than the O-atoms, the oxygen sputter rate is higher and the surface becomes niobium rich. The investigated samples consist of a $Pt\text{-}Nb_2O_5\text{-}Pt$ stack. The oxide layer was irradiated by different Ar-doses before top electrode deposition. At the highest dose Φ = 3e16 cm^{-2} the resulting oxygen gradient enables resistive switching.

[1] Bertaud et al. (TSF 520, 2012)
[2] Mähne et al. (MEMCOM Workshop 2012)

DS 34.8 Fri 11:30 H32

Multilevel resistive switching in Ar+ irradiated BiFeO3 thin films

— •Yao Shuai[1], Xin Ou[2], Wenbo Luo[2], Nan Du[3], Danilo Bürger[2,3], Oliver G. Schmidt[3,4], and Heidemarie Schmidt[3] — [1]State Key Laboratory of Electronic Thin Films and Integrated Devices, UESTC, China — [2]Helmholtz-Zentrum Dresden-Rossendorf e.V., Institute of Ion Beam Physics and Materials Research, Germany — [3]University of Technology Chemnitz, Faculty of Electrical Engineering and Information Technology, 09107 Chemnitz, Germany — [4]Institute for Integrative Nanosciences, IFW Dresden, Helmholtzstraße 20, 01069 Dresden, Germany

Low energy Ar+ ion irradiation has been applied to an Au/BiFeO3/Pt capacitor structures before deposition of the Au top electrode. The irradiated thin films exhibit multilevel resistive switching without detrimental resistance degradation, which makes the intermediate resistance states more distinguishable as compared to the non-irradiated thin film [1]. The stabilization of resistance states after irradiation is discussed based on the analysis of conduction mechanism during the resistive switching in BiFeO3 with a rectifying Au top electrode and a nonrectifying Pt bottom electrode [2]. Furthermore, it is shown how the conduction mechanisms change from room temperature to 423 K. [1] Y. Shuai, X. Ou et al., IEEE Device Letters, 2012, in press. [2] Y. Shuai, S. Zhou, D. Bürger, M. Helm, H. Schmidt, J. Appl. Phys. 109 (2011), 124117-4.

DS 34.9 Fri 11:45 H32

Influence of thickness ratio on resistive switching in BiFeO3:Ti/BiFeO3 bilayer structures

— •Tiangui You[1], Wenbo Luo[2], Yao Shuai[1,2], Nan Du[1], Danilo Bürger[1,3], Ilona Skorupa[3], Oliver G. Schmidt[1,4], and Heidemarie Schmidt[1] — [1]Chemnitz University of Technology, 09107 Chemnitz, Germany — [2]University of Electronic Science and Technology of China, 610054 Chengdu, China — [3]Helmholtz-Zentrum Dresden-Rossendorf, P.O. Box 510119, 01314 Dresden, Germany — [4]IFW-Dresden, 01069 Dresden, Germany

Nonvolatile resistive switching in BiFeO3 (BFO) [1] has attracted increasing attention; however, the underlying resistive switching mechanism is still controversial which restricts its application in nonvolatile memory devices. BFO:Ti/BFO bilayer structures with a 540 nm thick BFO layer and different thickness of BFO:Ti layer were grown on Pt/Sapphire substrates by pulsed laser deposition using the same growth conditions. Circular Au top electrodes were prepared with magnetron sputtering. Au/BFO/Pt single layer structures show a symmetric I-V curve without hysteresis due to the formation of Schottky contacts at both the top and bottom interface. However, Au/BFO/BFO:Ti/Pt bilayer structures exhibit an obvious resistive switching behavior under both voltage polarities. The influence of the thickness of BFO:Ti on the conduction mechanisms in Au/BFO/BFO:Ti/Pt bilayer structures is discussed to reveal similarities and differences between single and bilayer structures.

Reference [1] Y. Shuai et al., J. Appl. Phys., 109, 124117(2011)

DS 34.10 Fri 12:00 H32

Nanoscale resistive switching in epitaxial and polycrystalline BiFeO3 thin films

— •Yao Shuai[1], Wenbo Luo[1], Chuangui Wu[1], Wanli Zhang[1], Oliver G. Schmidt[2,3], and Heidemarie Schmidt[2] — [1]State Key Laboratory of Electronic Thin Films and Integrated Devices, UESTC, China — [2]University of Technology Chemnitz, Faculty of Electrical Engineering and Information Technology, 09107 Chemnitz, Germany — [3]Institute for Integrative Nanosciences, IFW Dresden, 01069 Dresden, Germany

Nonvolatile [1], bipolar, and multilevel [2] resistive switching has been observed in ca. 500 nm thick polycrystalline BiFeO3 thin films with rectifying, circular Au top electrodes and a nonrectifying Pt bottom electrode. The diameter of the Au top electrodes amounts to ca. 0.5 mm. By scanning a positionable top contact with a diameter of only 10 nm over polycrystalline BiFeO3 thin films under a constant applied dc voltage, the high and low resistance state can be locally written and afterwards read. It has been observed that for thinner polycrystalline BiFeO3 films with a thickness below 300 nm, no resistive switching can be observed either with large or with small scale top contacts. Bipolar resistive switching can also be realized in ca. 50 nm thick epitaxial BiFeO3 films on SrRuO3/SrTiO3 with a positionable top contact. This resistance is mainly determined by the ferroelectric polarization and the barrier height of the top and bottom contact. For thicker epitaxial BiFeO3 films the unique relation between ferroelectric polarization and resistance state is diminished. [1] Y. Shuai et al., J. Appl. Phys. 109 (2011). [2] Y. Shuai et al., IEEE Device Letters (2012) in press.

DS 34.11 Fri 12:15 H32

An electronic implementation of amoeba anticipation

— •Mirko Hansen[1], Karlheinz Ochs[2], Martin Ziegler[1], and Hermann Kohlstedt[1] — [1]Faculty of Engineering, Christian-Albrechts-Universität zu Kiel, 24143 Kiel, Germany — [2]Ruhr-Universität Bochum, 44780 Bochum, Germany

In nature, the capability to memorize environmental changes can already be observed in unicellular organisms like amoebas[1]. An amoeba changes its locomotive speed when it is exposed to unfavorable conditions. If a series of unfavorable conditions is applied, the amoeba later on behaves similarly on a single incident. Pershin et al.[2] are able to emulate this behavior using a simple resistive switching circuit model consisting of an inductor, a capacitor and a resistive switching device. We experimentally implement this model using a resistive switching device. A theoretical analysis of the circuit is presented to gain further insight into the functionality of this model and to give advice for the implementation of resistive switching devices in LC-circuits.

[1] T. Saigusa, A. Tero, T. Nakagaki, Y. Kuramoto, Phys. Rev. Lett. **100**, (2008) 018101

[2] Y. V. Pershin, S. La Fontaine, M. Di Ventra, Phys. Rev. E **80**, (2009) 021926

DS 34.12 Fri 12:30 H32

Lattice dynamics in Sb- and Te-based phase-change materials

— •Ronnie Ernst Simon[1,2], Ilya Sergueev[3], and Raphaël Pierre Hermann[1,2] — [1]Jülich Centre for Neutron Science JCNS and Peter Grünberg Institut PGI, Jara-FIT Forschungszentrum Jülich GmbH, D-52425 Jülich, Germany — [2]Faculté des Sciences, Univer- sité de Liège, B-4000 Liège, Belgium — [3]Deutsches Elektronen- Syn- chrotron, D-22607 Hamburg, Germany

Phase-change materials exhibit a significant change of the optical reflectivity and electrical resistivity upon crystallization which renders these materials applicable for optical storage devices and non-volatile electronic memories. In order to understand the switching kinetics between the amorphous and the metastable crystalline states a detailed knowledge of the lattice dynamics of the different phases is crucial. A suitable technique for the investigation of lattice dynamics is nuclear inelastic scattering (NIS) which gives access to the element specific density of phonon states (DPS). We performed NIS measurements in Sb- and Te-based phase-change materials in the amorphous and crystalline phases. We have recently extended the experimental possibilities by demonstrating the feasibility of high pressure NIS measurements, up to 75 GPa, in Sb_2Te_3 . The ESRF is acknowledged for the provision of synchrotron radiation beamtime at ID18.

DS 35: Application of Thin Films

Time: Friday 9:30–12:00 Location: H8

DS 35.1 Fri 9:30 H8

Aperiodic multilayer mirrors for attosecond water window pulses — •Alexander Guggenmos[1,2], Roman Rauhut[1,2], Michael Hofstetter[1,2], Samira Hertrich[3], Bert Nickel[3], Eric M. Gullikson[4], Ferenc Krausz[1,2], and Ulf Kleineberg[1,2] — [1]Ludwig-Maximilians-Universität München, Fakultät für Physik, Garching, Germany — [2]Max-Planck-Institut für Quantenoptik, Garching, Germany — [3]Ludwig-Maximilians-Universität München, Fakultät für Physik, München, Germany — [4]Center for X-Ray Optics, Lawrence Berkeley National Lab, Berkeley, USA

Attosecond pulses pave the way towards the direct observation of electron dynamics in atoms, molecules or solid surfaces with an unprecedented temporal precision. Chirped broadband multilayer mirrors are key components to shape these pulses generated from high harmonic radiation facilitating an even deeper physical insight into these dynamics by compressing high harmonic pulses to their fourier limit utilizing short pulse pump-probe experiments. Aperiodic broadband multilayer XUV mirrors exhibit the required degree of freedom for tailored shaping of attosecond pulses. Extending the current technology to the water window spectral range around 300-500 eV requires multilayer optics of atomic precision since the spectral phase is extremely sensitive to even smallest thickness errors. We will present the investigations of chirped aperiodic multilayer XUV optics for the water window range with atomic precision to control spectral and temporal features. Furthermore simulations and optimizations of multilayer systems as well as experimental results of XRR and XUV measurements are presented.

DS 35.2 Fri 9:45 H8

Hard x-ray focusing below 10 nm by multilayer zone plates fabricated by the combination of pulsed laser deposition and focused ion beam — •Florian Döring[1], Christian Eberl[1], Tobias Liese[1], Felix Schlenkrich[1], Volker Radisch[1], Hans-Ulrich Krebs[1], Anna-Lena Robisch[2], Markus Osterhoff[2], Sarah Hoffmann[2], Matthias Bartels[2], and Tim Salditt[2] — [1]Institut für Materialphysik, University of Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany — [2]Institut für Röntgenphysik, University of Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

In hard x-ray microscopy, one approach for point transmission focusing is to use of multilayer zone plates instead of conventional Fresnel zone plates, which are difficult to prepare with high aspect ratio. Therefore, aperiodic W/Si multilayers were pulsed laser deposited (PLD at 248 nm) with high quality on a W wire with single layer thicknesses according to the zone plate law (width of smallest layer Δr = 5.2 nm). Then, from the coated wires, a lens was fabricated by cutting, transferring on a W-tip and polishing using focused ion beam (FIB). X-ray focusing experiments were performed at the coherence beamline P10 of Petra III, showing a far-field pattern which exhibits the expected high numerical aperture. Measured far-field pattern, the corresponding autocorrelation of the focal intensity distribution as well as a three plane iterative phase reconstruction of the zone plate exit wave are in agreement with a focal width in between 6 and 10nm (FWHM), which compares well with the expected 1.22 Δr = 6.3 nm.

DS 35.3 Fri 10:00 H8

Interface investigation of ion-beam deposited Chromium/ Scandium multilayer mirrors — •Roman Rauhut[1,2], Alexander Guggenmos[1,2], Samira Hertrich[3], Bert Nickel[3], Sriram Venkatesan[4], Christina Scheu[4], Eric M. Gullikson[5], Ferenc Krausz[1,2], and Ulf Kleineberg[1,2] — [1]Ludwig-Maximilians-Universität München, Fakultät für Physik, Garching, Germany — [2]Max-Planck-Institut für Quantenoptik, Garching, Germany — [3]Ludwig-Maximilians-Universität München, Fakultät für Physik, München, Germany — [4]Ludwig-Maximilians-Universität München, Fakultät für Chemie, München, Germany — [5]Center for X-Ray Optics, Lawrence Berkeley National Lab, Berkeley, USA

The direct observation of electron dynamics in atoms, molecules or on surfaces with a unprecedented temporal precision requires attosecond pulses from High Harmonic Generation (HHG) sources. Shaping, filtering and steering these pulses requires highly efficient XUV optics based in many cases on multilayer mirror technology. This leads to the necessity of developing as perfect interfaces as possible, due to the huge loss in reflectivity from boundary imperfections. We will present a systematic optimization of ion-beam deposited Cr/Sc multilayer mirrors by a variation of ion beam voltages during the deposition process as well as the application of ion-assisted deposition, which leads to the fabrication of highly reflecting multilayer optics in the water window. Experimental results from X-ray reflectometry, spectral ellipsometry and XUV reflectometry measurements as well as TEM cross section images are shown and discussed.

DS 35.4 Fri 10:15 H8

Temperature and bias voltage induced electron tunneling through ultrathin TaOx barriers. — •Ievgen Nedrygailov[1], Katrin Asteman[2], Eckart Hasselbrink[1], and Detlef Diesing[1] — [1]Fakultät für Chemie, Universität Duisburg-Essen, D-45117 Essen, Germany — [2]Heraeus Precious Metals GmbH & Co. KG, Conductive Polymer Division (Clevios), Chempark Leverkusen, 51368 Leverkusen, Germany

The ability to control tunneling of electrons through ultrathin (1-5 nm) dielectric films is a prerequisite for high-performance metal-insulator-metal (MIM) structures. Due to the nonlinear current-voltage characteristics and ultrafast transport of charge carriers through the built-in potential barrier these structures are widely used in nanoelectronic applications such as single electron transistors, thermometers, coolers, radiation and chemically excited hot charge carriers (chemicurrents) detectors.

In this contribution we discuss the use of Pt-TaOx-Ta structures for detection of chemicurrents under elevated temperature conditions, which are typical for higher pressure catalysis. We focus on the separation of the current of hot charge carriers and secondary effects, such as the current induced by the temperature difference across the tunnel junction or by an applied bias voltage. Possible advantages of ultrathin MIM structures over metal-semiconductor detectors, which are commonly used in chemicurrent studies, are also discussed.

DS 35.5 Fri 10:30 H8

Effect of composition and strain on conductivity of $LaNiO_3$ thin films — Mingwei Zhu[1,2], •Philipp Komissinskiy[1], Aldin Radetinac[1], Mehran Vafaee[1], and Lambert Alff[1] — [1]Department of Materials Science, Technische Universität Darmstadt, 64287 Darmstadt, Germany — [2]Shenyang National laboratory for Materials Science, Institute of Metal Research, Chinese Academy of Sciences, Wenhua Road 72, 110016 Shenyang, People's Republic of China

Highly conductive oxide $LaNiO_3$ (LNO) is an excellent electrode material for all-oxide electronic devices. We have grown 35-50 nm thick $La_{1+x}Ni_{1-x}O_3$ thin films by pulsed laser deposition. Fine tuning of the Ni/La ratio in the films is achieved by using targets with various cation stoichiometry x = 0.04, 0.01, -0.09 as measured by energy dispersive spectrometry. We observe that the conductivity of the LNO films can be controlled by tailoring the Ni/La ratio. The LNO films deposited using a target with slight excess of Ni show record low resistivity values of about 80 $\mu\Omega \cdot cm$ at room temperature. The excess Ni oxidizes to NiO as evident from X-ray diffraction measurements. The effect of compressive and tensile strain on conductivity was studied using LNO films grown on $SrTiO_3$, $LaAlO_3$, $LaSrAlO_4$, and $(La,Sr)(Al,Ta)O_3$ substrates. This work was supported by the National Natural Science Foundation of China (No.51202256) and China Scholarship Council (CSC)

DS 35.6 Fri 10:45 H8

Growth of highly conductive $SrMoO_3$ as lattice matched oxide electrode material for (Ba,Sr)TiO_3 based thin film heterostructures — •Aldin Radetinac, Jürgen Ziegler, Mehran Vafaee, Philipp Komissinskiy und Lambert Alff — Materialwissenschaften, Technische Universität Darmstadt, Petersenstraße 23, 64287 Darmstadt, Germany

We have grown epitaxial heterostructures of $Ba_{0.6}Sr_{0.4}TiO_3$ and $SrMoO_3$ [1] by pulsed laser deposition on $SrTiO_3$ (001) substrates. A 5 nm thick interlayer of $Ba_{0.6}Sr_{0.4}TiO_{3-\delta}$ grown at low oxygen pressures and flow prevents oxidation of the conducting $SrMoO_3$ bottom electrode. Beneath this capping layer, a Mo^{4+} valence state fraction of 80% is maintained even after oxygen annealing as observed by X-ray photoelectron spectrometry (XPS). The described oxygen interface engineering allows fully epitaxial growth of the heterostructure enabling the future use of the novel highly conductive electrode material $SrMoO_3$ e.g. in tunable varactors.

This work was supported by the DFG projects GRK 1037 (TICMO) and KO 4093/1-1.

[1] A. Radetinac, K. S. Takahashi, L. Alff, M. Kawasaki, and Y. Tokura, Appl. Phys. Express **3**, 073003(2010).

DS 35.7 Fri 11:00 H8

Chemical purity in high performance solution processed zinc oxide TFTs — •Marlis Ortel, Torsten Balster, and Veit Wagner — Research Center for Functional Materials and Nanomolecular Science, Jacobs University Bremen, Campus Ring 1, 28759 Bremen, Germany

Conversion of precursor materials in solution processed semiconductor plays an important role in device application. The organic by-products from zinc acetate conversion into ZnO have a significant influence on the electronic structure of the resulting semiconductor layer. They can significantly influence charge transport in the material. Hence the impact of deposition and post-deposition annealing on the chemical composition of the ZnO semiconductor was investigated by means of x-ray photoelectron spectroscopy (XPS), optical and electrical measurements in a wide process temperature range from 200°C to 500°C. It was found, that the increase in deposition temperature from 360°C to 500°C leads to a reduction in carbon content by 30% and an increase of the oxygen to zinc ratio from 0.82 to 0.96. These XPS results correspond well with optical measurements, which exhibit a blue-shift of the optical band gap by 20 meV to a value of 3.19 eV reflecting an improved layer quality. The layers were electrically analyzed in a field-effect transistor geometry. The optimization in the purity of the ZnO semiconductor by thermal treatment lead to an improvement of the field-effect mobility up to $13cm^2V^{-1}s^{-1}$. The increase in mobility is found to be correlated to an on-set voltage shift from 14V to an ideal value of 0V, which reflects a reduction in the level of deep traps.

DS 35.8 Fri 11:15 H8

Retention of Ferroelectric VDF-TrFE Copolymer Thin Films Characterized by Nondestructive Polarization Readout — •Danny von Nordheim[1], Sebastian Koch[1], Soichiro Okamura[2], and Bernd Ploss[1] — [1]Department of SciTec, University of Applied Sciences Jena, Carl-Zeiss-Promenade 2, 07745 Jena, Germany — [2]Department of Applied Physics, Tokyo University of Science, Shinjuku, Tokyo 162-8601, Japan

Usual retention tests are based on the application of read pulses to a ferroelectric sample while the charge response is recorded. These tests, however, do not allow the continuous recording of retention as after the application of the read pulse the ferroelectric is in a new state defined by the sign of the read pulse. We propose a novel approach which is based on the nondestructive readout of the remanent polarization by measurement of small signal dielectric nonlinearities. The temporal development of the remanent polarization is directly accessible from the measured first and second harmonics in the current response to a small sinusoidal voltage signal. The novel technique has been used to investigate the retention of thin VDF-TrFE copolymer films of molar ratio 70/30 with thickness below 200 nm. This technique may also be useful for the nondestructive readout of ferroelectric memory cells. Compared to the destructive readout by polarization switching the rewrite of the initial polarization is not required and the lifetime of the memory cell increased.

DS 35.9 Fri 11:30 H8

The Co2p spin and oxidation state in Co-PI catalysts — •Matthias Richter and Dieter Schmeisser — Brandenburg University of Technology Cottbus, Applied Physics and Sensors, K.-Wachsmann-Allee 17, 03046 Cottbus, Germany

The electronic structure of cobalt based catalysts used for photocatalytic water splitting in solar cells is analyzed using synchrotron radiation photoelectron spectroscopy. The catalyst films are prepared by electrochemical deposition. We employ a X-ray photoelectron spectroscopy study to analyze the Co2p and O1s core levels, absorption edges and valence bands. We discuss our resonant data in terms of the partial density of states of the valence and conduction band. We find a difference in the Co oxidation state as a function of film thickness (deposited charge). From the relative amount of Co, O, K and P we favor the molecular cobaltate cluster-like structure as the structural motif of the Co-PI catalyst. Further, at resonant PES at the Co2p edge we find the Co2p partial DOS to exhibit no sharp features next to the VBM, instead there is a broad emission at around 6eV below E_{Fermi}. The former are found in $LiCoO_2$ and other Co-oxide systems with a Co^{3+} ground state. We attribute such sharp features to the low spin (LS) configuration of Co^{3+} and deduce that in the Co catalysts there is no evidence for the corresponding LS contributions. Our data prove the Co^{2+} ground state and demonstrate that it is exclusively in the $Co3d^7$ high spin state in the pristine catalyst films.

DS 35.10 Fri 11:45 H8

Epitaxial Ag: Opening Doors to New Opportunities in Plasmonics — •Charlotte E. Sanders[1], Bo-Hong Li[2], Chih-Kang Shih[1], and Xianggang Qiu[2] — [1]The University of Texas at Austin, Department of Physics, Austin, TX U.S.A. — [2]Chinese Academy of Sciences, Beijing National Laboratory for Condensed Matter Physics and Institute of Physics, Beijing, China

It has been shown that noble metals can grow epitaxially on semiconducting and insulating substrates: although such films constitute non-wetting systems, low temperature deposition followed by room temperature annealing leads to atomically flat film. We recently made a major breakthrough with the demonstration of the superiority of epitaxial Ag as a low-loss plasmonics platform in the visible regime, and with the harnessing of the special plasmonic properties of Ag for plasmonic nanolasing (Science 337, 450 (2012)). Now we have extended our investigation to the infrared regime, where we have measured extraordinary optical transmission through arrays of subwavelength-diameter perforations in order to compare the strength of plasmonic resonances in epitaxial Ag film with those in polycrystalline Ag film grown by thermal evaporation. Our results suggest (in agreement with simulation and with our previous findings in the visible regime) that the high losses and short propagation distances that until now have been typical in surface plasmon studies are due largely to scattering from the surface roughness characteristic of thermally evaporated polycrystalline films. These results, newly published in Nano Letters (doi:10.1021/nl303029s), will be elaborated upon in this presentation.