Thin Films Division
Fachverband Dünne Schichten (DS)

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Overview of Invited Talks and Sessions

(lecture rooms H2 and H8; poster A and D1)

Gaede Prize

DS 20.1	Wed	14:00–14:45	H36	**Photonic Metamaterials: Novel Optics with Artificial Atoms** — •Stefan Linden

Invited Talks

DS 12.1	Tue	9:30–10:15	H8	**Preparation methods and thermoelectric properties of PbTe based nanocomposites containing an inclusion phase** — Denis Petri, Christoph Erk, •Sabine Schlecht, Ralf Hassdorf, Eckhard Müller, Gert Homm, Markus Piechotka, Florian Gather, Peter J. Klar
DS 18.1	Wed	9:30–10:15	H2	**X-ray Scattering Investigations of Ge Quantum-dot Crystals Depositied on Prepatterened Si Substrates** — •Vaclav Holý, M. Mixa, J Stangl, T. Fromherz, R. T. Lechner, E. Wintersberger, G. Bauer, Ch. Dais, E. Müller, D. Grützmacher
DS 21.1	Wed	15:00–15:45	H2	**Self-organization of noble-metal nanoparticles on rippled dielectric surfaces produced by low-energy ion erosion** — •David Babonneau, Sophie Camelio, Lionel Simonot
DS 30.1	Thu	9:30–10:15	H2	**Spin in organics, a new route to spintronics** — •Bert Koopmans
DS 32.1	Thu	14:00–14:45	H2	**Spintronics below one nanometer** — •Laurent Limot
DS 34.1	Thu	16:15–17:00	H2	**Probing the structure and dynamics of biomolecules adsorbed on surfaces.** — •Peter Weightman
DS 42.1	Fri	10:15–11:00	H2	**A molecular view of the interfaces of colloidal particles and nanoscopic oil droplets in water** — •Sylvie Roke

Invited talks of the joint symposium SYDF – Density Functional Theory and Beyond for Real Materials

See SYDF for the full program of the Symposium.

SYDF 1.1	Thu	14:45–15:15	H1	**Downfolded Self-Energy of Many-Electron Systems and the Hubbard U** — •Ferdi Aryasetiawan
SYDF 1.2	Thu	15:15–15:45	H1	**LDA+Gutzwiller method for correlated electron systems** — •Zhong Fang
SYDF 1.3	Thu	15:45–16:15	H1	**Localized and itinerant states in d/f-electron systems unified by GW@LDA+U** — •Hong Jiang
SYDF 1.4	Thu	16:30–17:00	H1	**Giant polaronic effects in solids and nanstructures** — •Andrea Marini
SYDF 1.5	Thu	17:00–17:30	H1	**Excitation energies with time-dependent density *matrix* functional theory** — •Evert Jan Baerends, Klaas J. H. Giesbertz, Oleg Gritsenko, Katarzyna Pernal
SYDF 1.6	Thu	17:30–18:00	H1	**Calculations of multipoles in magnetic metals and insulators** — •Lars Nordström

Invited talks of the joint symposium SYNT – Nanotribology

See SYNT for the full program of the Symposium.

SYNT 1.1	Fri	10:15–10:45	H1	**Atomic friction under ultrahigh vacuum conditions** — •Ernst Meyer, Enrico Gnecco, Pascal Steiner, Gregor Fessler, Sascha Koch, Thilo Glatzel, Alexis Baratoff, Mircin Kisiel, Urs Gysin, Akshata Rao, Shigeki Kawai, Sabine Maier
SYNT 1.2	Fri	10:45–11:15	H1	**Layering and Squeeze-out Damping in Confined Liquid Films** — •Frieder Mugele
SYNT 1.3	Fri	11:15–11:45	H1	**Wear on the nanoscale: mechanisms and materials** — •Bernd Gotsmann, Mark A. Lantz, Harish Bhskaran, Abu Sebastian, Ute Drechsler, Michel Despont, Yun Chen, Kumar Sridharan, Papot Jaroenapibal, Robert Carpick
SYNT 1.4	Fri	11:45–12:15	H1	**Friction at the Nanoscale: Insights from Atomistic Simulations** — •Izabela Szlufarska, Yifei Mo, Yun Liu, Maneesh Mishra
SYNT 1.5	Fri	12:15–12:45	H1	**The friction of wrinkles** — •Martin H. Müser, Hamid Mohammadi
SYNT 1.6	Fri	12:45–13:15	H1	**Influence of humidity on nano- and micromechanical contact adhesion** — •Hans-Jürgen Butt

Invited talks of the joint symposium SYGN – Spin-Orbit Coupling and Spin Relaxation in Graphene and Carbon Nanotubes

See SYGN for the full program of the Symposium.

SYGN 1.1	Mon	14:00–14:35	H1	**Models for spin-orbit coupling in graphene** — •Francisco Guinea
SYGN 1.2	Mon	14:35–15:10	H1	**Spin-orbit coupling and spin relaxation in carbon nanotube quantum dots** — •Ferdinand Kuemmeth
SYGN 1.3	Mon	15:10–15:45	H1	**Spin-orbit interaction in carbon nanotubes probed in pulsed magnetic fields** — •Sungho Jhang, Magdalena Marganska, Yurii Skourski, Dominik Preusche, Benoit Witkamp, Milena Grifoni, Herre van der Zant, Joachim Wosnitza, Christoph Strunk
SYGN 1.4	Mon	16:00–16:35	H1	**Wigner molecules and spin-orbit coupling in carbon-nanotube quantum dots** — •Massimo Rontani
SYGN 1.5	Mon	16:35–17:10	H1	**Spin relaxation and decoherence in graphene quantum dots** — •Guido Burkard
SYGN 1.6	Mon	17:10–17:45	H1	**Spin transport in graphene field effect transistors** — •Bart van Wees

Invited talks of the joint symposium SYPN – Polarization Field Control in Group III-Nitrides

See SYPN for the full program of the Symposium.

SYPN 1.1	Thu	9:30–10:00	H1	**Growth and applications of N-polar (Al,Ga,In)N** — •Stacia Keller, Umesh K Mishra
SYPN 1.2	Thu	10:00–10:30	H1	**Green light-emitting diodes and laser heterostructures on semi-polar GaN(11-22)/sapphire substrates** — •Andre Strittmatter
SYPN 1.3	Thu	10:30–11:00	H1	**Pros and cons of green InGaN lasers on polar GaN substrates** — •Uwe Strauss, Adrian Avramescu, Teresa Lermer, Jens Müller, Christoph Eichler, Stephan Lutgen
SYPN 1.4	Thu	11:15–11:45	H1	**Molecular beam epitaxy as a method for the growth of free-standing zinc-blende GaN layers and substrates.** — •Sergei Novikov, Thomas Foxon, Anthony Kent
SYPN 1.5	Thu	11:45–12:15	H1	**Three-dimensional GaN for semipolar light emitters** — •Thomas Wunderer, Frank Lipski, Stephan Schwaiger, Ferdinand Scholz, Martin Feneberg, Klaus Thonke, Andrey Chuvilin, Ute Kaiser, Sebastian Metzner, Frank Bertram, Jürgen Christen, Clemens Vierheilig, Ulrich Schwarz

Topical Talks

DS 1.1	Mon	10:15–10:45	H2	**Tunable Hollow Waveguides and Their Device Applications** — •Fumio Koyama
DS 1.2	Mon	10:45–11:15	H2	**Self-organized quantum dots as single and entangled photon emitters** — •Erik Stock, Waldemar Unrau, Anatol Lochmann, Jan Amaru Töfflinger, Andrei Schliwa, Irina Ostapenko, Murat Öztürk, Sven Rodt, Till Warming, Askhat K. Bakarov, Aleksandr I. Toropov, Ilia A. Derebezov, Vladimir Haisler, Dieter Bimberg
DS 1.3	Mon	11:15–11:45	H2	**Nanostructures for Novel Quantum Cascade Structures** — •K. Unterrainer, W. Parz, T. Moldaschl, A. Benz, G. Fasching, A.M. Andrews, G. Strasser
DS 1.4	Mon	11:45–12:15	H2	**Quantum dot single-photon sources** — •Peter Michler
DS 1.5	Mon	12:15–12:45	H2	**The Two Conflicting Narratives of Metal-Optics** — •Eli Yablonovitch
DS 1.6	Mon	12:45–13:15	H2	**Fundamental formulation of nanoplasmonic lasers** — •Shun Chuang
DS 2.1	Mon	14:00–14:30	H2	**High performance lasers realised by advanced nanofabrication technologies** — •Johann Peter Reithmaier
DS 2.2	Mon	14:30–15:00	H2	**High-brightness edge-emitting semiconductor lasers based on concepts of photonic band crystal and titled wave lasers** — •Vladimir Kalosha, Thorsten Kettler, Kristian Posilovic, Daniel Seidlitz, Vitaly Shchukin, Nikolay Ledentsov, Dieter Bimberg
DS 2.3	Mon	15:00–15:30	H2	**Semiconductor optical amplifiers (SOA) for linear and nonlinear applications** — •Wolfgang Freude, René Bonk, Thomas Vallaitis, Andrej Marculescu, Amita Kapoor, Christian Meuer, Dieter Bimberg, Romain Brenot, François Lelarge, Guang-hua Duan, Juerg Leuthold
DS 2.4	Mon	15:30–16:00	H2	**Controlling light on the Nanoscale** — •Nikolay Zheludev
DS 2.5	Mon	16:15–16:45	H2	**New developments of high power LEDs and challenges in lighting applications** — •Christian Fricke
DS 2.6	Mon	16:45–17:15	H2	**High speed VCSELs for short reach DATACOM applications** — •Alex Mutig, James Lott, Sergey Blokhin, Gerrit Fiol, Alexey Nadtochiy, Vitaly Shchukin, Nikolai Ledentsov, Dieter Bimberg
DS 2.7	Mon	17:15–17:45	H2	**Long-Wavelength Vertical-Cavity Surface-Emitting Lasers with a High-Contrast Grating** — •Werner Hofmann
DS 14.1	Tue	14:00–14:30	H8	**Thermal Conductivity of Thermoelectric Materials Embedded with Nanoparticles** — •Yee Kan Koh, David Cahill
DS 19.1	Wed	10:30–11:00	H2	**Glancing angle deposition: Preparation, properties, and application of micro- and nanostructured thin films** — •Bernd Rauschenbach, Christian Patzig, Jens Bauer, Chinmay Khare
DS 19.7	Wed	12:15–12:45	H2	**Synthesis of Nanostructured Films by Self-organization** — •Hans Hofsäss
DS 22.1	Wed	16:00–16:30	H2	**Self-organization during the growth of phase-separated nanostructured thin films** — •Gintautas Abrasonis
DS 22.5	Wed	17:15–17:45	H2	**Self-organization and molecular diffusion processes in organic thin film growth** — •Christian Teichert
DS 31.1	Thu	10:30–11:00	H2	**Spintronics with Organic Semiconductors** — •V. Alek Dediu
DS 31.2	Thu	11:00–11:30	H2	**Muon measurements of spin transport and dynamics in organic semiconductors** — •Alan Drew
DS 31.6	Thu	12:15–12:45	H2	**Role of the van der Waals interaction on the adsorption of organic molecules on surfaces** — •Nicolae Atodiresei
DS 33.1	Thu	15:00–15:30	H2	**Spin-dependent tunneling through a single molecule with intramolecular resolution** — •Roland Wiesendanger
DS 33.2	Thu	15:30–16:00	H2	**Tunneling through magnetic molecules: what can we learn from the master equation?** — •Carsten Timm, Florian Elste, Binhe Wu
DS 35.1	Thu	17:15–17:45	H2	**Surface enhanced infrared spectroscopy - pushing the detection limit towards zeptomolar sensitivity** — •Frank Neubrech, Daniel Weber, Jörg Bochterle, Annemarie Pucci
DS 35.5	Thu	18:30–19:00	H2	**Infrared spectroscopic ellipsometry for the in-situ investigation of responsive polymer brushes** — •Dennis Aulich, Eva Bittrich, Klaus-Jochen Eichhorn, Petra Uhlmann, Manfred Stamm, Martin Brücher, Roland Hergenröder, Olha Hoy, Igor Luzinov, Norbert Esser, Karsten Hinrichs
DS 43.1	Fri	11:15–11:45	H2	**High resolution studies of bio-molecules using TERS** — •Volker Deckert

DS 43.4	Fri	12:15–12:45	H2	**Molecular orientation in phthalocyanine films assessed by combined optical and magneto-optical investigations** — •Georgeta Salvan, Michael Fronk, Björn Bräuer, Dietrich R. T. Zahn, Oliver G. Schmidt, Jens Kortus
DS 43.8	Fri	13:30–14:00	H2	***In-silico* optimization of function and emissive properties of Silicon nanoparticles** — •Thomas Niehaus

Sessions

DS 1.1–1.6	Mon	10:15–13:15	H2	**Nanophotonics - Devices I (Focused Session together with HL)**
DS 2.1–2.7	Mon	14:00–17:45	H2	**Nanophotonics - Devices II (Focused Session together with HL)**
DS 3.1–3.9	Mon	10:15–12:30	H8	**Organic Electronics and Photovoltaics I (Joint Session DS/CPP/HL/O)**
DS 4.1–4.6	Mon	14:00–15:30	H8	**Organic Electronics and Photovoltaics II (Joint Session DS/CPP/HL/O)**
DS 5.1–5.6	Mon	15:45–17:15	H8	**Nanoengineered Thin Films**
DS 6.1–6.7	Mon	16:00–17:45	H15	**[HL] Organic Semiconductors: Solar Cells (Joint Session DS/CPP/HL/O)**
DS 7.1–7.9	Mon	10:15–12:45	H3	**[MA] Multiferroics I (Joint Session of MA/DF/KR/DS)**
DS 8.1–8.14	Mon	14:00–17:45	H3	**[MA] Multiferroics II (Joint Session of MA/DF/KR/DS)**
DS 9.1–9.53	Mon	15:00–17:30	Poster D1	**Poster: Synthesis of Nanostructured Films by Self-organization, Thermoelectric Thin Films and Nanostructures, High-k and Low-k Dielectrics, Layer Deposition Processes, Layer Growth, Layer Properties, Application of Thin Films, Surface Modification, Hard and Superhard Coatings, Metal Layers**
DS 10.1–10.10	Tue	10:30–13:00	H2	**Plasmonics and Nanophotonics I (Joint Session DS/O/HL)**
DS 11.1–11.6	Tue	15:00–16:30	H2	**[O] Plasmonics and Nanophotonics II (Joint Session DS/O/HL)**
DS 12.1–12.1	Tue	9:30–10:15	H8	**Invited Schlecht**
DS 13.1–13.10	Tue	10:30–13:00	H8	**Thermoelectric Thin Films and Nanostructures I**
DS 14.1–14.5	Tue	14:00–15:30	H8	**Thermoelectric Thin Films and Nanostructures II**
DS 15.1–15.12	Tue	9:30–12:45	H15	**[HL] Organic Semiconductors: Transistors and OLEDs (Joint Session DS/CPP/HL/O)**
DS 16.1–16.12	Tue	9:30–12:45	H37	**[CPP] Organic Electronics and Photovoltaics I (Joint Session DS/CPP/HL/O)**
DS 17.1–17.10	Tue	13:45–16:15	H37	**[CPP] Organic Electronics and Photovoltaics II (Joint Session DS/CPP/HL/O)**
DS 18.1–18.1	Wed	9:30–10:15	H2	**Invited Holý**
DS 19.1–19.7	Wed	10:30–12:45	H2	**Synthesis of Nanostructured Films by Self-organization I (Focused Session)**
DS 20.1–20.1	Wed	14:00–14:45	H36	**Gaede-Prize Talk (Linden, Stefan)**
DS 21.1–21.1	Wed	15:00–15:45	H2	**Invited Babonneau**
DS 22.1–22.5	Wed	16:00–17:45	H2	**Synthesis of Nanostructured Films by Self-organization II (Focused Session)**
DS 23.1–23.6	Wed	9:30–11:00	H8	**High-k and Low-k Dielectrics I (Joint Session DS/DF)**
DS 24.1–24.6	Wed	11:15–12:45	H8	**High-k and Low-k Dielectrics II (Joint Session DS/DF)**
DS 25.1–25.4	Wed	16:00–17:00	H8	**Application of Thin Films**
DS 26.1–26.12	Wed	9:30–12:45	H37	**[CPP] Organic Electronics and Photovoltaics III (Joint Session DS/CPP/HL/O)**
DS 27.1–27.11	Wed	10:30–13:15	H32	**[O] Plasmonics and Nanooptics III (Joint Session DS/O/HL)**
DS 28.1–28.11	Wed	15:00–17:45	H32	**[O] Plasmonics and Nanooptics IV (Joint Session DS/O/HL)**
DS 29.1–29.56	Wed	15:00–17:30	Poster A	**Poster: Molecular Spintronics, Biomolecular and Functional Organic Layers, Organic Electronics and Photovoltaics, Plasmonics and Nanophotonics, Organic Thin Films, Nanoengineered Thin Films, Thin Film Characterisation,**
DS 30.1–30.1	Thu	9:30–10:15	H2	**Invited Koopmans**
DS 31.1–31.6	Thu	10:30–12:45	H2	**Molecular Spintronics - Current Status and Challenges I (Focused Session)**

DS 32.1–32.1	Thu	14:00–14:45	H2	**Invited Limot**
DS 33.1–33.2	Thu	15:00–16:00	H2	**Molecular Spintronics - Current Status and Challenges II (Focused Session)**
DS 34.1–34.1	Thu	16:15–17:00	H2	**Invited Weightman**
DS 35.1–35.5	Thu	17:15–19:00	H2	**Biomolecular and Functional Organic Layers I (Focused Session)**
DS 36.1–36.6	Thu	9:30–11:00	H8	**Thin Film Characterisation: Structure Analyse and Composition (XRD, TEM, XPS, SIMS, RBS, ...) I**
DS 37.1–37.6	Thu	11:15–12:45	H8	**Thin Film Characterisation: Structure Analyse and Composition (XRD, TEM, XPS, SIMS, RBS, ...) II**
DS 38.1–38.11	Thu	14:00–16:45	H8	**Layer Properties: Electrical, Optical and Mechanical Properties**
DS 39.1–39.4	Thu	17:00–18:00	H8	**Layer Deposition Processes & Layer Growth**
DS 40.1–40.10	Thu	10:30–13:00	H32	**[O] Plasmonics and Nanooptics V (Joint Session DS/O/HL)**
DS 41.1–41.12	Thu	15:00–18:00	H32	**[O] Plasmonics and Nanooptics VI (Joint Session DS/O/HL)**
DS 42.1–42.1	Fri	10:15–11:00	H2	**Invited Roke**
DS 43.1–43.8	Fri	11:15–14:00	H2	**Biomolecular and Functional Organic Layers II (Focused Session)**
DS 44.1–44.6	Fri	10:15–11:45	H8	**Organic Thin Films I**
DS 45.1–45.4	Fri	12:00–13:00	H8	**Organic Thin Films II**
DS 46.1–46.9	Fri	14:00–16:15	H8	**Organic Thin Films III**
DS 47.1–47.7	Fri	11:15–13:00	H32	**[O] Plasmonics and Nanooptics VII (Joint Session DS/O/HL)**
DS 48.1–48.6	Fri	11:15–12:45	H40	**[O] Organic Electronics and Photovoltaics III (Joint Session DS/CPP/HL/O)**

Annual General Meeting of the German Vacuum Society (DVG)

Monday 17:30–18:00 H8

Annual General Meeting of the Thin Films Division (DS)

Monday 18:00–18:30 H8

DS 1: Nanophotonics - Devices I (Focused Session together with HL)

Time: Monday 10:15–13:15 Location: H2

Topical Talk DS 1.1 Mon 10:15 H2

Tunable Hollow Waveguides and Their Device Applications — •Fumio Koyama — P&I Laboratory, Tokyo Institute of Technology, 4259-R2-22, Nagatsuta, Midori-ku, Yokohama 226-8503, Japan

We proposed a tunable hollow optical waveguide with a variable air core toward a new class of photonic integrated circuits. We present various unique features in hollow waveguides and the combination with microelectro-mechanical system (MEMS). We describe the design and fabrication of tunable hollow waveguides with a variable air core. We demonstrated low loss and polarization insensitive waveguides. The result shows a possibility of a giant change of over $\sim 10\%$ in propagation constant with a variable air core. We also present a wide variety of device applications based on hollow waveguides, which include tunable Bragg reflectors, tunable lasers, dispersion compensators and so on. In particular, a hybrid-integrated tunable in-plane laser based on HCG-DBR hollow waveguide was demonstrated. A giant tuning range of 52 nm in wavelength has been demonstrated with SMSR of 30 dB. An expected advantage of HWG laser can be its athermal operation resulting from the air-core guiding. A fully monolithic version of the presented device with MEMS tuning can solve alignment issues to offer further large tuning range. Their simplicity and scalability may open up applications in large-scale photonic integration and in realizing other optical functions.

Topical Talk DS 1.2 Mon 10:45 H2

Self-organized quantum dots as single and entangled photon emitters — •Erik Stock[1], Waldemar Unrau[1], Anatol Lochmann[1], Jan Amaru Töfflinger[1], Andrei Schliwa[1], Irina Ostapenko[1], Murat Öztürk[1], Sven Rodt[1], Till Warming[1], Askhat K. Bakarov[2], Aleksandr I. Toropov[2], Ilia A. Derebezov[2], Vladimir Haisler[2], and Dieter Bimberg[1] — [1]Institut für Festkörperphysik, TU-Berlin, 10623 Berlin, Germany — [2]Institute of Semiconductor Physics, 630090 Novosibirsk, Russia

The development of semiconductor based single photon and entangled photon emitters with high efficiency will be a fundamental element for quantum key distribution systems. We have developed InGaAs/GaAs quantum dot (QD) based Resonant-Cavity LEDs (RC-LED). The resonant cavity leads to an increased external quantum efficiency and due to the Purcell effect to an increased spontaneous emission rate allowing us to electrically pump the single QD at 1 GHz repetition rate.

The biexciton-exciton recombination cascade can be used for the generation of entangled photon pairs, if the finestructure splitting (FSS) of the exciton bright states is less than the homogenous line width. Using 8-band $k \cdot p$ theory we predict that symmetric QDs grown on (111) GaAs substrate will demonstrate a vanishing FSS. Mikrophotoluminescence spectroscopy on single QDs grown on (111) GaAs demonstrates a FSS < 10 μeV limited by the spectral resolution of our setup. This work was partly funded by the SFB 787 and the SfP 982735.

Topical Talk DS 1.3 Mon 11:15 H2

Nanostructures for Novel Quantum Cascade Structures — •K. Unterrainer, W. Parz, T. Moldaschl, A. Benz, G. Fasching, A.M. Andrews, and G. Strasser — Photonik Institut und Zentrum für Mikro&Nanostrukturen, Technische Universität Wien, A-1040 Wien

In this contribution we will discuss carrier relaxation in quantum wells and quantum dots and its importance for THz quantum cascade lasers (QCLs). THz QCLs have shown rapid improvements of their emission power and wavelength control. However, the operation temperature is still limited to cryogenic temperatures. All attempts to overcome this limitation involve the control of carrier relaxation. Optical phonon relaxation together with other elastic processes determine the non-radiative recombination. We use time-resolved near-infrared pump and THz probe experiments to study carrier dynamics and find that carrier-carrier scattering causes fast relaxation in quantum wells. The subsequent reduction of the doping concentration in QCLs has led to considerably reduced threshold currents. However, the temperature performance has only increased marginal. A further reduction of scattering is only possible by reducing the phase space. As a first step, we have applied a strong magnetic field causing in-plane quantization. The emission intensity of THz QCLs as function of the applied magnetic field shows an increase of the emission power and a decrease of the threshold. Thus, quantum dots should improve the performance of QCLs significantly. We investigate carrier relaxation between sub-levels and study the design requirements for quantum dot cascade structures.

Topical Talk DS 1.4 Mon 11:45 H2

Quantum dot single-photon sources — •Peter Michler — Institut für Halbleiteroptik und Funktionelle Grenzflächen, Universität Stuttgart, 70569 Stuttgart, Allmandring 3, Germany

Exploiting the quantum properties of the light which is emitted from semiconductor nanostructures has the potential of enabling many new applications in the field of photonics and quantum information technology, such as secure communication, imaging and lithography techniques beyond the diffraction limit, as well as photonic quantum computing. Many of these applications require the generation of triggered single photons or even indistinguishable photons. Single quantum dots in microcavities open this possibility. In my talk, I will discuss the fascinating physic as well as the current status of such light sources.

Topical Talk DS 1.5 Mon 12:15 H2

The Two Conflicting Narratives of Metal-Optics — •Eli Yablonovitch — University of California, Berkeley, CA 94720, USA

There are two conflicting narratives of Electromagnetics in metals:

1. The microwave circuit narrative in which metals, distributed capacitors, and distributed inductors function together in a high frequency circuit, albeit as distributed components. Here there is a rich tradition of various electromagnetic functions, including the antenna function.

2. This is countered by the optical-plasmonic narrative, in which metallic electromagnetics is thought to be dominated by plasmons, electromagnetic normal modes in which the inertia of the electrons plays a major role.

Given that Electromagnetics is generally invariant with frequency, it is not clear why there need to be two separate narratives. Is metal-optics simply the high frequency version of microwave electromagnetics? There is great benefit in unifying our understanding of the two regimes of metallic electromagnetics, and to distinguish the occasional role of electron inertia.

We find that some of the most important metal-optics functions are best understood as extensions of microwave electromagnetics: Antennas, for example, have been thoroughly under-estimated, and are well-poised to change the rules of optical physics.

Topical Talk DS 1.6 Mon 12:45 H2

Fundamental formulation of nanoplasmonic lasers — •Shun Chuang — University of Illinois, Department of Electrical and Computer Engineering, 1406 West Green Street, Urbana, Illinois, 61801, USA

The smallest laser conventionally requires an optical cavity with a size of one half of the effective wavelength in all three directions, which is often referred as the diffraction limit of the cavity. To make a laser with an active volume smaller than the diffraction limit, an idea is to surround the optical waveguide with metals. In this case, the effective volume of the optical mode can be significantly reduced in spite of a higher intrinsic absorption due to the metal loss at optical frequencies. By placing the active materials such as quantum dots or quantum wells near the region of peak optical field, it is possible to enhance the spontaneous and stimulated emissions to overcome the intrinsic loss from metals.

In this talk, we will present a fundamental formulation for nanoplasmonic lasers, which accounts for the negative permittivity and dispersion of metal plasma in a nanocavity. We point out the importance of using the energy (instead of power) confinement factor. We then discuss the ideas of a Fabry-Perot type of plasmonic waveguide laser and a nano-bowtie optical antenna coupled to semiconductor quantum dots, which function as the gain medium.

DS 2: Nanophotonics - Devices II (Focused Session together with HL)

Time: Monday 14:00–17:45 Location: H2

Topical Talk DS 2.1 Mon 14:00 H2

High performance lasers realised by advanced nanofabrication technologies — •Johann Peter Reithmaier — Institute of Nanostructure Technologies and Analytics, Kassel, Germany

With advanced nanofabrication techniques beyond conventional semiconductor fabrication technologies, one has access to more independent parameters for the optimization of the device performance or the fabrication process itself. Two major nanostructure technologies will be addressed in this talk. One is based on self-organized growth of quantum dot materials with new formation techniques and structure designs, which are used for the realization of temperature stable high power lasers. Recent device results, e.g. based on tunnel-injection structures, and the realization of coolerless pump modules will be discussed. The second technique is based on nanolithography and high aspect ratio dry-etching, which allows the fabrication of surface defined gratings for high-speed multi-section DFB and DBR lasers. Recent results of such devices fabricated with this low-cost nanoimprint compatible fabrication technology will be presented. The work was mainly performed in the frame of two European projects (Brighter, DeLight).

Topical Talk DS 2.2 Mon 14:30 H2

High-brightness edge-emitting semiconductor lasers based on concepts of photonic band crystal and titled wave lasers — •Vladimir Kalosha, Thorsten Kettler, Kristian Posilovic, Daniel Seidlitz, Vitaly Shchukin, Nikolay Ledentsov, and Dieter Bimberg — Institute for Solid-State Physics, Technical University Berlin, Berlin, Germany

We will report on current status of the design, fabrication and performance of edge-emitting waveguide lasers and their arrays which are based on concepts of photonic band crystal (PBC) lasers and tilted wave lasers (TWL). Such lasers provide high radiation power and low beam divergence and present potentially a new elementary basis for high-brightness laser systems. Following to PBC concept, the laser is formed by multiple quasi-periodic AlGaAs layers and varying height and width of multiple stripes. As compared to typical lasers, they are characterized by an extremely large mode area and provide discrimination of high-order modes. Experimentally we have obtained a brightness of 8.7×10^7 W/cm^2/sr in pulsed regime and vertical and lateral beam quality factor $M^2 < 2$ for large range of the pump current in pulsed and cw regimes at 980 nm. Maximum power of 3.5, 10.5 and 27 W was achieved for one, three-and nine-stripe lasers, scalable with the number of stripes. Following to the TWL concept, the laser is formed by coupled narrow and broad waveguides and give rise in ultra-narrow tilted beam from the broad waveguide at proper phase-matching. Experiments have demonstrated far-field divergence of TWLs well below 1° and improved wavelength stability in wide pumping ranges.

Topical Talk DS 2.3 Mon 15:00 H2

Semiconductor optical amplifiers (SOA) for linear and nonlinear applications — •Wolfgang Freude[1], René Bonk[1], Thomas Vallaitis[1], Andrej Marculescu[1], Amita Kapoor[2], Christian Meuer[3], Dieter Bimberg[3], Romain Brenot[4], François Lelarge[4], Guang-hua Duan[4], and Juerg Leuthold[1] — [1]Inst. of Photonics and Quantum Electronics, Karlsruhe Institute of Technology, Germany — [2]On leave from Shaheed Rajguru College of Appl. Sciences for Women, Delhi, India — [3]Inst. of Solid State Physics, TU Berlin, Germany — [4]Alcatel-Thalès III-V Lab, Palaiseau, France

SOA characteristics for two selected applications are discussed, namely linear in-line amplification in gigabit passive optical networks (GPON), and fast nonlinear all-optical signal processing. As linear amplifiers, SOA feature moderate cost, low energy needs, $10\ldots25\,$dB gain in a bandwidth of $60\ldots120\,$nm, and a peak-gain range of $1.25\ldots1.60\,\mu$m.

In all-optical fast signal processing, SOA serve as regenerative wavelength converters, as nonlinear elements for four-wave mixing, and as switches. The respective application areas are determined by the SOA parameters gain, saturation power, recovery time, α-factor and noise figure.

Quantum-dot (QD) SOA are known for pattern-free amplification and fast cross-gain modulation. We demonstrate that QD SOA are also well suited as linear in-line amplifiers because of their large saturation power, wide dynamic range, large burst mode tolerance and small cross-phase modulation (XPM) due to a low α-factor. On the other hand, bulk SOA can be engineered for low saturation power and large α-factor, which enables nonlinear signal processing via XPM.

Topical Talk DS 2.4 Mon 15:30 H2

Controlling light on the Nanoscale — •Nikolay Zheludev — University of Southampton, UK

We overview recent results on ultrafast active plasmonics, nanoscale phase change photonics, nonlinear and switchable metamaterials and tuneable free-electron light source on a chip.

15 min Coffee Break

Topical Talk DS 2.5 Mon 16:15 H2

New developments of high power LEDs and challenges in lighting applications — •Christian Fricke — Neophos Development Pte. Ltd, Jocherstr.7, 85221 Dachau

Improvement of PowerLED structures is still at a tremendous improvement rate per year. Epitaxy, chip design, phosphor efficiency and package design see large improvements - The brightness of LED devices increased by a factor of 4 over the last 4 years and will certainly continue over the next years. Light quality and device cost for LEDs that are to be marketed for home and office lighting are key to successfully replace conventional lighting by LED solutions. Only when standardized modular systems are available to the market consumers will switch at an accelerated rate. Key performance indicators will be presented as well as an outlook to individual tunable light sources fitting to existing home / office installations.

Topical Talk DS 2.6 Mon 16:45 H2

High speed VCSELs for short reach DATACOM applications — •Alex Mutig[1], James Lott[2], Sergey Blokhin[1], Gerrit Fiol[1], Alexey Nadtochiy[1], Vitaly Shchukin[3], Nikolai Ledentsov[2], and Dieter Bimberg[1] — [1]Institut für Festkörperphysik und Zentrum für Nanophotonik, Technische Universität Berlin, Hardenbergstrasse 36, 10623 Berlin, Federal Republic of Germany — [2]VI Systems GmbH, Hardenbergstrasse 7, 10623 Berlin, Federal Republic of Germany — [3]PBC Laser GmbH, Hardenbergstrasse 36, 10623 Berlin, Federal Republic of Germany

Around the year 2001 VCSELs emerged as the key component for up to 10 Gbit/s, aggregated high speed local-area and storage-area network data communication systems and soon thereafter for optical cable links for computer and consumer applications as well. The rapid increase in serial transmission speed and the limitations of copper wire-based links at bit rates >10 Gbit/s and distances >1 m greatly expanded the possible application areas of fiber-optic interconnects. Here we present our work on oxide-confined VCSELs operating at bit rates up to 40 Gbit/s and at low current densities of $\sim$10 kA/cm^2, sufficient for reliable operation. The small signal modulation bandwidths and resonant frequencies up to $\sim$22 GHz are measured, and the relaxation resonance frequency, damping factor, and electrical parasitic cut-off frequency are evaluated. According to our results with further improvement in the device design to reduce parasitics optical modulation bandwidths exceeding 30 GHz can be realized, leading toward reliable VCSEL serial operation at rates up to 50 Gbit/s.

Topical Talk DS 2.7 Mon 17:15 H2

Long-Wavelength Vertical-Cavity Surface-Emitting Lasers with a High-Contrast Grating — •Werner Hofmann — Technische Universität Berlin

Long-wavelength Vertical-Cavity Surface-Emitting Lasers (VCSELs) based on a subwavelength high-contrast gratings (HCGs) as output mirrors have been realized for the first time. By design, these devices are highly polarization stable, single-mode at large apertures and solve the VCSEL-mirror problem at long wavelengths in an elegant way. The device is grown on an InP substrate, incorporating a BTJ for a low electrical and optical losses and avoiding p-material. A hybrid reflector is used as bottom-mirror and the light is coupled out via the HCG reflector. With cost effective mass-fabrication in mind, the top HCG reflector consists of amorphous silicon on isolator. The single-mode laser emission is tailored to be around 1320 nm wavelength targeting applications in high-speed optical data transmission, especially for passive optical networks. The device is manufactured in a low parasitics, high-speed design, good for bandwidths well above 10 GHz. We report single-mode emission for devices with apertures as large as 11 μm operating continuous wave with output-powers in excess of 0.4 mW. Pulsed operation with output powers up to 4 mW at room temperature is demonstrated as well. This is the first electrically pumped VCSEL structure realized in this wavelength regime utilizing an HCG mirror.

DS 3: Organic Electronics and Photovoltaics I (Joint Session DS/CPP/HL/O)

Time: Monday 10:15–12:30 Location: H8

DS 3.1 Mon 10:15 H8

Colour tuneable light-emitting transistor — •Eva J. Feldmeier, Christian Melzer, and Heinz von Seggern — Electronic Materials Department, Institute of Materials Science Technische Universität Darmstadt, Petersenstraße 23, 64287 Darmstadt, Germany

In recent years the interest in ambipolar organic light-emitting field-effect transistors has increased steadily as the devices combine switching behaviour of transistors with light emission. Usually, small molecules and polymers with a band gap in the visible spectral range serve as semiconducting materials. Mandatory remain balanced injection and transport properties for both charge carrier types to provide full control of the spatial position of the recombination zone of electrons and holes in the transistor channel via the applied voltages. As will be presented here, the spatial control of the recombination zone opens new possibilities towards light-emitting devices with colour tuneable emission.

In our contribution an organic light-emitting field-effect transistors is presented whose emission colour can be changed by the applied voltages. The organic top-contact field-effect transistor is based on a parallel layer stack of acenes serving as organic transport and emission layers. The transistor displays ambipolar characteristics with a narrow recombination zone within the transistor channel. During operation the recombination zone can be moved by a proper change in the drain and gate bias from one organic semiconductor layer to another one inducing a change in the emission colour. In the presented example the emission maxima can be switched from 530 nm to 580 nm.

DS 3.2 Mon 10:30 H8

Improved transport properties of p-i-i small molecule solar cells deposited on heated substrates — •Steffen Pfuetzner, Karl Leo, and Moritz Riede — Institut für Angewandte Photophysik, Technische Universität Dresden

To achieve higher efficiencies in organic solar cells, ideally the open circuit voltage (V_{OC}), fill factor (FF) as well as the short current density (j_{SC}) have to be improved further. However, in bulk heterojunction (BHJ) solar cells jsc and the FF are typically limited by charge carrier recombination due to transport problems (e.g. low mobility, dead ends) in the BHJ. A suitable way to modify the BHJ layer morphology and to improve solar cell parameters is substrate heating during bulk layer deposition. Furthermore, j_{SC} can be enhanced by replacing C_{60} by C_{70}. We show that substrate heating at 90°C leads to improved FF and j_{SC} for a C_{60} and ZnPc containing BHJ solar cell with the following stack structure: ITO/p-Di-NPD/C_{60}:ZnPc/C_{60}/BPhen/Al. However, in case of similar C_{70}:ZnPc solar cells, no significant improvements are observed. Using SEM we show that the preferential aggregation by heating is completely suppressed by the p-doped underlayer Di-NPD. To force aggregation of the heated C_{70}:ZnPc bulk, 5 nm intrinsic ZnPc layer is deposited on the p-Di-NPD layer and verified by SEM. J-V characteristics show a drop in FF and Voc with the additional interlayer ZnPc. To overcome this problem probably caused by transport barriers to the neighboring layers, experiments with doped ZnPc are carried out.

DS 3.3 Mon 10:45 H8

Analysis of Chemical Degradation Mechanism of Phosphorescent Organic Light Emitting Devices by Laser-Desorption/Ionization Time-of-Flight Mass Spectrometry — •Ines Rabelo de Moraes, Sebastian Scholz, Björn Lüssem, and Karl Leo — Institut für Angewandte Photophysik, Technische Universität Dresden, George-Bähr-Str. 1, 01062 Dresden, Germany

Phosphorescent Organic Light Emitting diodes (OLEDs) have attracted much interest for their potential application in full color flat-panel displays and as an alternative lighting source. However, low efficiency, and the short operation lifetime, in particular in the case of blue emitting devices, are the major limitations for the current OLEDs commercialization. In order to overcome these limitations, a deep knowledge about the aging and the degradation mechanism is required [1]. Our work focuses on the chemical degradation mechanism of different iridium based emitter materials like FIrpic (light blue) and Ir(ppy)3 (green), commonly used in OLEDs. For this purpose, the devices were aged by electrical driving until the luminance reached 6% of the initial luminance. The laser-desorption/ionization time-of-flight mass spectrometry was used to determine specific degradation pathways.

[1] Hany Aziz, and Zoran D. Popovic, Chem. Mater. 16, 4522 (2004).

DS 3.4 Mon 11:00 H8

Spatially resolved, polarization dependent absorption and photocurrent measurements of pentacene based OFETs — •Christian Westermeier, Matthias Fiebig, and Bert Nickel — Department für Physik and CeNS, Ludwig-Maximilians-Universität, Geschwister-Scholl-Platz 1, 80539 München

Pentacene is a promising candidate for organic electronics and optoelectronic applications due to its high charge carrier mobility and strong absorption properties. Forming a triclinic herringbone structure, its optical properties are highly anisotropic [1]. Pentacene films show a thin-film-phase texture. The grains inducing the texture should absorb linear polarised light depending on their orientation with respect to the direction of polarisation.

Here we use local illumination of the transistor channel in a confocal laser scanning setup with a spatial resolution in the submicron regime [2]. The pentacene grains in the channel of our OFETs exhibit a size of a few microns in diameter. The absorption of separate grains is found to be strongly dependent on the polarisation of the incident light, as expected. Thus, the scanning technique allows for imaging of grain orientation with a submicron resolution over large areas.

Absorption being the initialising step to generate excitons is important for optoelectronic devices like solar cells and the photoresponse of transistors. The influence of polarisation on the spatially resolved photocurrent of pentacene OFETs will be discussed.

[1] M. Dressel, et al., Opt. Express 16, 19770-19778 (2008)

[2] M. Fiebig, et al., Appl. Phys. A 95, 1, 113-117 (2009)

DS 3.5 Mon 11:15 H8

In-situ Analysis of Charge Carrier Mobility in Field Effect Transistors During Organic Semiconductor Deposition — •Christopher Keil, Dominik Klaus, Jan Hartel, and Derck Schlettwein — Institute of Applied Physics, Justus-Liebig-University Giessen, Germany. email:schlettwein@uni-giessen.de

Films of $F_{16}PcCu$ prepared by physical vapour deposition under high vacuum conditions were characterized in situ during the growth from the monolayer range up to about 100 nm. The charge carrier mobility in the linear and saturation region as well as the threshold voltage were investigated in real time at deliberate film thickness by help of a real time analysis software routine. The organic films were deposited on thermally grown silicon oxide which also acts as gate dielectric. The underlying Si wafer served as a bottom gate electrode and structured inter-digital metal source- drain contacts were prepared by photolithography. Different channel lengths and widths as well as different metal contacts were used to determine the influence of semiconductor/metal contacts on the characteristics of the field effect transistors.

DS 3.6 Mon 11:30 H8

Investigation of contact properties of organic field effect transistors — •M. Grobosch[1], I. Hörselmann[2], S. Scheinert[2], M. Knupfer[1], and G. Paasch[1] — [1]IFW Dresden, D-01069 Dresden, Germany — [2]Technical University Ilmenau, D-98684 Ilmenau, Germany

Source/drain contacts in OFETs based on a solution prepared modified P3HT were characterized by combined X-ray and ultra violet photoemission spectroscopy (XPS, UPS) and electrical measurements of the OFET whereas the sample preparation for the different measuring principles has been realized in parallel differing in the layer thickness of the polymer. By means of UPS a reduced work function could be demonstrated for different prepared, sputtered, and as-received Au contacts in agreement with previous publications. Furthermore the chemistry and the electronic structure of the interfaces between Au metal deposited onto thin films of solution prepared modified P3HT on sputtered Au contacts have been studied. From the observed well defined molecular orbitals we have found an interface dipole of +1.5 eV and a hole injection barrier of about 0.6 eV. However, one cannot expect such a high barrier from the measured characteristics of the OFET because the currents are not contact limited. Clarifying the reason for such a discrepancy we have carried out two-dimensional simulations. These results confirm clearly for a barrier of 0.6 eV strongly reduced drain currents would be measured. The difference in the layer thickness can be the reason for the measured difference but further investigations are necessary to explain more in detail this phenomenon.

DS 3.7 Mon 11:45 H8

Improving the mobility of the CuPc OFETs by variing the substrate preparation — •Iulia G. Korodi[1], Daniel Lehmann[1], Michael Hietschold[2], and Dietrich R. T. Zahn[1] — [1]Semiconductor Physics, Chemnitz University of Technology, D-09107 Chemnitz, Germany — [2]Solid Surfaces Analysis Group, Chemnitz University of Technology, D-09107 Chemnitz, Germany

Top-contact organic field-effect transistors (OFETs) using Copper Phthalocyanine (CuPc) as active layer were produced under high vacuum conditions ($p \leq 5 \times 10^{-7}$ mbar). 20 nm thick organic films were deposited by Organic Molecular Beam Deposition on highly p-doped Si(100) substrates with 100 nm SiO_2 as the gate dielectric. Source and drain electrodes of gold were deposited through a shadow mask on top of the organic layer with the substrate cooled by liquid nitrogen.

The performance of the OFETs was tested in vacuum as well as in atmosphere. The highest mobility of CuPc OFETs was found to be $\mu_{vacuum} = (1.5 \pm 0.6)\,10^{-3}\,\mathrm{cm}^2/\mathrm{Vs}$. When the substrate was modified by applying an elevated temperature (130 °C) during deposition of the CuPc film the mobility of the OFETs increased by a factor of ≈ 6. The threshold voltage was also improved from a value of $V_{Th} = -(15.0 \pm 0.3)$ V to $V_{Th} = -(9.6 \pm 1.4)$ V for deposition at room and elevated substrate temperatures, respectively. A similar effect on the electrical characteristics was found after modifying the gate dielectric with a self-assembled monolayer of n-octadecyltrichlorosilane. The improved OFET performance with the variation of the substrate conditions will be discussed.

DS 3.8 Mon 12:00 H8

Electrical characterization of operating OFETs using Kelvin Probe Force Microscopy — •Franziska Lüttich, Harald Graaf, Iulia G. Korodi, Daniel Lehmann, Dietrich R. T. Zahn, and Christian von Borczyskowski — Center for nanostructured Materials and Analytics, Chemnitz University of Technology, Germany

We present recent results on n-type organic field effect transistors (OFETs) using Atomic Force Microscopy (AFM) and Kelvin Probe Force Microscopy (KPFM). These studies allow the local potential in the channel of OFETs during operation to be determined. The transistor structures investigated differ in gate insulator treatment and substrate temperature during evaporation of the organic material.

All investigated top-contact OFETs were fabricated under high-vacuum conditions ($p < 4 \cdot 10^{-7}$ mbar) by evaporating PDI8-CN_2 on top of a p-doped silicon substrate covered by a SiO_2 layer. Gold-electrodes were evaporated through a shadow mask on top of the organic layer. The gate insulator modification was implemented prior to the substrate transfer into the vacuum chamber. For this purpose monolayers of N-octadecyltrichlorosilane (OTS) resulting in hydrophobic surfaces were employed. In the case of deposition at elevated temperature the substrate was kept at 130°C.

These variations of preparation influence the structural and electronic properties of the OFET and result in changes of the charge carrier mobility. The effects observed indicate tuning possibilities for organic devices leading to increased charge carrier mobility.

DS 3.9 Mon 12:15 H8

Experimental study and time dependent modeling of OFETs with solid electrolyte gate dielectrics — •Katharina Schätzler[1], Klaus Schmidt[1], Walter Fix[1], Gottfried Döhler[1], and Heiko Weber[2] — [1]PolyIC GmbH & Co. KG, Fürth — [2]Lehrstuhl für Angewandte Physik, Friedrich-Alexander-Universität, Erlangen

We successfully investigated and simulated organic field effect transistors (OFETs) with a solid organic insulator containing ionic salt. It is already well known that electrolytes as gate dielectrics in OFETs offer low operating voltages by means of a high capacitance. Hence, the charge carrier density is increased in the channel region of the semiconductor. However, the drain-source current I_{ds} shows a strong time dependency because of the limited mobility of the ions. Consequently we developed a time dependent model for the spatial distribution of the ionic current within the insulator matrix. The ionic current of both cations and anions splits in a diffusion and a drift process. The model very precisely reproduces the time as well as the ion concentration dependency of I_{ds}. Parameters like ion and semiconductor mobility are extracted and are in good agreement with parameters extracted from experimental OFET and capacitance characteristics.

DS 4: Organic Electronics and Photovoltaics II (Joint Session DS/CPP/HL/O)

Time: Monday 14:00–15:30 Location: H8

DS 4.1 Mon 14:00 H8

Influence of the substrate-lattice-geometry on the island shape of organic thin films — •M. Benedetta Casu[1], Britt-E. Schuster[1], Indro Biswas[1], Christoph Raisch[1], Helder Marchetto[2], Thomas Schmidt[2], T. Onur Menteş[3], Miguel A. Nino[3], Andrea Locatelli[3], and Thomas Chassé[1] — [1]IPTC, University of Tübingen, Tübingen, Germany — [2]Fritz-Haber-Institut, Berlin, Germany — [3]Sincrotrone Trieste S.C.p.A., Trieste, Italy

By using a combination of microscopic imaging and diffraction techniques with structural and chemical sensitivity, we studied the growth of diindenoperylene (DIP) on Au(100), and Au(111). Growth and structure of DIP films of different thickness were monitored in situ including real time PEEM and LEEM performed at the beamlines Nanospectroscopy at Elettra, and UE49-PGM-b-SMART at BESSY. A layer-by-layer mechanism characterizes the initial growth in both cases followed by island nucleation, i.e., the growth follows the Stranski-Krastanov mode. The islands surprisingly show a fractal-like shape when the DIP thin films are deposited on a Au(111) single crystal. DIP thin films deposited on various substrates at RT have been investigated, revealing the tendency to Stranski-Krastanov growth but the observed islands were always compact (i.e. non-fractal). In particular, real time LEEM investigations on Au(100), under the same preparation conditions as on Au(111), show compact islands. We interpret the fractal growth of DIP for these kinetic growth conditions as a consequence of the triangular symmetry of the substrate, as seen in homoepitaxial and heteroepitaxial metal on metal growth.

DS 4.2 Mon 14:15 H8

Can X-ray microspectroscopy probe inhomogeneities in the electron structure of organic devices? — •Christian Hub, Martin Burkhardt, Marcus Halik, and Rainer Fink — Interdisciplinary Center for Molecular Materials (ICMM), Universität Erlangen, Egerlandstraße 3, 91058 Erlangen, Germany

The degree of homogeneity in the morphology of organic thin film devices has a major impact on the charge transport properties. Real devices usually strongly deviate from the ideal device structure since epitaxial growth with low defect concentrations cannot be achieved. We have recently started to investigate pentacene-based OFETs, which were prepared using commercial silicon nitride membranes as dielectric showing excellent transport characteristics. The overall device thickness is sufficiently small to perform scanning transmission X-ray microspectroscopy (SXTM) experiments at the PolLux microspectroscope. Grains with varying preferential orientation in the polycrystalline pentacene films are detected using the significant local NEX-

AFS dichroism. The local NEXAFS contrast is utilized to investigate differences in the electronic structure within these films while the devices are operated. Using the standard photomultiplier tube of the PolLux as detector no pronounced changes were observed when current is driven through the organic films. Therefore electron detection was implemented to further enhance the sensitivity of the microscope to ultrathin films. We will discuss the related problems and opportunities to use local NEXAFS with lateral resolution below 30 nm. The work is funded by the BMBF under contract 05 KS7WE1.

DS 4.3 Mon 14:30 H8

Morphology and electronic properties of an electron acceptor adsorbed on organic insulator pre-covered metal surfaces — •P. Amsalem[1], J. Frisch[1], A. Wilke[1], A. Vollmer[2], R. Rieger[3], K. Müllen[3], J.-P. Rabe[1], and N. Koch[1] — [1]Humboldt-Universität zu Berlin, Institut für Physik, Brook-Taylor-Str. 6, 12489 Berlin, Germany — [2]HZB-BESSY II, Albert-Einstein-Str. 15, 12489 Berlin, Germany — [3]Max Planck Institut für Polymerforschung, Ackermannweg 10, 55128 Mainz, Germany

In this work, we explore the possibility of tuning the interface energetics at a pi-conjugated (electron acceptor) molecule-metal interface by modifying the adsorbate-substrate distance through pre-adsorption of insulating organic monolayers. We report a photoemission study of the growth of hexaazatriphenylene-hexacarbonitrale (HATCN) deposited on N,N-bis-(1-naphthyl)-N,N-diphenyl1-1,1-biphenyl1-4,4-diamine(α-NPD) or tris(8-hydroxyquinoline)aluminum (Alq$_3$) pre-covered Ag(111) surfaces. α-NPD and Alq$_3$ are known to be weakly adsorbed on Ag(111) and have both been used as thin organic spacer. The choice of HATCN has been motivated by its high electronic affinity ($\sim$3.5 eV). HATCN molecules deposited on α-NPD/Ag(111) are found to diffuse below the α-NPD molecules pre-adsorbed on Ag(111). In the case of HATCN on Alq$_3$/Ag(111), an interface state close to the Fermi-level is observed. This interface state differs markedly from the one measured for HATCN in direct contact with Ag(111). The results are discussed in terms of the formation of polaronic states and charge transfer across insulating layers.

DS 4.4 Mon 14:45 H8

Energy levels and work function of ultra-thin polythiophene films on conductive polymer electrodes — •Johannes Frisch[1], Antje Vollmer[2], Jürgen P. Rabe[1], and Norbert Koch[1] — [1]Humboldt-Universität zu Berlin, Institut f. Physik, Brook-Taylor-Straße 6, D-12489 Berlin — [2]Elektronenspeicherring BESSY II, Albert-Einstein-Str. 15, D-12489 Berlin

In modern organic photovoltaic cells (OPVCs), poly(ethylene-dioxythiophene):poly(styrenesulfonate) (PEDT:PSS) and poly(3-hexylthiophene) (P3HT) are prototypical materials used as transparent anode and as donor polymer, respectively. In this context, it is essential to clarify how the efficiency of OPVCs based on these materials depends on the position of the energy level at the interface. In the present work, the morphology, work function, and energy level alignment of ultra-thin films of P3HT on PEDT:PSS were investigated using photoelectron spectroscopy (XPS, UPS). Ultra-thin films (down to sub-monolayer coverages) were produced by spin coating P3HT films on PEDT:PSS followed by a subsequent washing process. It has been found that the deposition of ultra-thin P3HT films on PEDT:PSS lowers the sample work function (Φ) by 0.4 eV due to doping of P3HT film with positive charges from the PEDT:PSS layer. The valence band edge (VBE) is located only 0.1 eV below the Fermi-level. For thicker P3HT films (ca. 10 nm), Φ further decreases by 0.2 eV and the VBE is observed 0.2 eV below the Fermi-level. These results are discussed within existing concepts of local work function fluctuations and energy level bending at the P3HT/PEDT:PSS interface.

DS 4.5 Mon 15:00 H8

Electronic properties of Cu-phthalocyanine-fullerene planar and bulk heterojunctions on PEDOT:PSS — •Andreas Wilke, Toshiko Mizokuro, Ralf Peter Blum, Jürgen P Rabe, and Norbert Koch — Institut für Physik, Humboldt-Universität zu Berlin, Brook-Taylor-Str. 6, D-12489 Berlin

In organic photovoltaic cells (OPVCs) typically two organic materials with electron-acceptor and electron-donor properties are placed between anode and cathode, forming either a layered planar or mixed bulk heterojunction where charge separation should occur. To improve the efficiency of this central process it is important to know and understand the energy levels at such heterojunctions, and how they may depend on heterojunction morphology. We report ultraviolet and X-ray photoelectron spectroscopy studies on layered planar and mixed bulk heterojunctions of Cu-phthalocyanine (CuPc) and C$_{60}$, a prototypical material pair for OPVCs. The respective heterojunctions were formed on poly(ethylene-dioxythiophene):poly(styrenesulfonate) substrates, in order to achieve morphologies comparable to those in actual OPVCs. The energy offset between the highest occupied levels of CuPc and C$_{60}$ was determined to 1.3 eV for both the layered and mixed bulk heterojunction. Our results demonstrate that the energy levels that determined the efficiency of charge separation in OPVCs made of CuPC and C$_{60}$ are independent of particular interface morphology, and that differences in device efficiency are due to other effects.

DS 4.6 Mon 15:15 H8

A high molecular weight donor for electron injection interlayers on metal electrodes — •Benjamin Bröker[1], Ralf-Peter Blum[1], Luca Beverina[2], Oliver T. Hofmann[3], Georg Heimel[1], Antje Vollmer[4], Johannes Frisch[1], Jürgen P. Rabe[1], Egbert Zojer[3], and Norbert Koch[1] — [1]Institut für Physik, Humboldt-Universität zu Berlin, Newtonstrasse 15, D-12389 Berlin, Germany — [2]Department of Materials Science and INSTM, State University of Milano-Bicocca, Via Cozzi 53,I-20125 Milano, Italy — [3]Institute of Solid State Physics, Graz University of Technology, Petersgasse 16, A-8010 Graz, Austria — [4]Helmholtz-Zentrum Berlin, Bessy II, Albert-Einstein-Str. 15, D-12489 Berlin, Germany

The molecular donor 9,9-ethane-1,2-diylidene-bis(N-methyl-9,10-dihydroacridine) (NMA) has been synthesized, and its electronic properties were characterized at interfaces to metals with photoelectron spectroscopy. Here a decrease of the sample work function is observed that becomes larger with increasing molecular coverage and clearly exceeds values that would be expected for metal surface electron "push back" alone, confirming the electron donating nature of NMA. For tris(8-hydroxyquinoline)aluminum (Alq$_3$) deposited on top of a NMA-modified Au(111) surface, the electron injection barrier (EIB) is reduced by 0.25 eV compared to that on pristine Au(111). Furthermore, the EIB reduction depends linearly on Θ of the donor-modified Au(111) surface, adjustable by NMA pre-coverage. Comparisons will also be given to the stronger donor MV0.
This work was supported by the EC project ICONTROL.

DS 5: Nanoengineered Thin Films

Time: Monday 15:45–17:15 Location: H8

DS 5.1 Mon 15:45 H8

Artificial granularity of two-dimensional arrays of nanodots prepared by electron-beam-induced-deposition (EBID) — •Fabrizio Porrati[1], Roland Sachser[1], Mike Strauss[2], Iryna Andrusenko[3], Tatiana Gorelik[3], Ute Kolb[3], and Michael Huth[1] — [1]Physikalisches Institut, Goethe-Universität, Frankfurt am Main — [2]MPI für Biophysik, Frankfurt am Main — [3]Institut für Physikalische Chemie, Gutemberg-Universität, Mainz

We have prepared 2D arrays of metallic nanodots embedded in an insulating matrix by means of EBID using the $W(CO)_6$ precursor. By varying the electron beam parameters, i.e. beam current and energy, and the array pitch we obtain granular media with tunable electrical properties. The analysis of the current-voltage characteristic suggests that the transport takes place by electron tunneling between the artificial grains. In order to understand the nature of the granularity and thus, the origin of the electron transport behaviour, we perform TEM and micro-Raman investigations. Independently of the deposition beam parameters, TEM measurements show that the dots are constituted by non-crystalline W-C clusters embedded in a non-crystalline carbonaceous matrix. Raman spectra show two peaks, around 690 cm^{-1} and 860 cm^{-1}, associated to W-C stretching modes, supporting the TEM data. Furthermore, the so called G and D peaks, at about 1560 cm^{-1} 1350 cm^{-1}, associated to vibration modes in disordered and amorphous carbon, are also detected. The analysis of the position of the peaks and of their relative intensity suggests that the microstructure of the matrix is between nanocrystalline and amorphous.

DS 5.2 Mon 16:00 H8

Strain-dependent conductivity of granular metals prepared by focused particle beam induced deposition — •Christina Grimm[1], Markus Baranowski[1], Friedemann Völklein[2], and Michael Huth[1] — [1]Physikalisches Institut, Goethe-Universität, D-60438 Frankfurt am Main, Germany — [2]Institut für Mikrotechnologien, Hochschule RheinMain, D-65428 Rüsselsheim, Germany

We report on the strain-dependence of the electrical conductivity of granular metals prepared by focused particle beam induced deposition. The samples were prepared in a dual-beam electron / Ga ion scanning microscope using selected precursors, such as $W(CO)_6$. Stripe-like deposits were fabricated on dedicated cantilevers pre-patterned with contact pads made from Cr/Au. The cantilever deflection was induced in-situ by means of a four axes nano-manipulator and the conductivity change was recorded by lock-in technique employing a Wheatstone resistance bridge. Current-voltage characteristics and strain-dependence were measured for samples of various thicknesses and composition. For selected samples time-dependent conductivity data were taken as the samples were slowly epxosed to air.

DS 5.3 Mon 16:15 H8

Direct comparision of large scale simulation of nanostructuring of metals with the experiment — •Dmitry Ivanov and Baerbel Rethfeld — TU-Kaiserslautern, Physcis Department, 67663

The process of short pulse laser nanostructuring of materials currently is a subject of active research interest from the side of rapidly progressive and promising scientific fields: IT- and BIO- technologies. The structures on sub wavelength scale obtained on metals [1] semiconductors [2] and insulators [3] exhibit unique properties from the point of both fundamental physics and possible technological applications. However, transient and nonequilibrium character of processes occurring simultaneously and on relatively wide time and spatial scales makes the experimental study limited and expensive on one hand and the applicability of the theoretical models difficult on the other one. In this work, the complete process of femtosecond laser nanostructuring of Au film on a substrate is modeled on the experimental scale in a super-large scale simulation based on Molecular Dynamics. [1] A.I. Kuznetsov, J. Koch, and B.N. Chichkov, Appl. Phys. A 94, 221 (2009). [2] J. Gottmann and R. Wagner, Proc. of SPIE 6106, 61061R (2006). [3] E. Akcöltekin, S. Akcöltekin, O. Osmani, A. Duvenbeck, H. Lebius and M. Schleberger, New J. of Phys. 10, 053007 (2008). [4] D.S. Ivanov, B.C. Rethfeld, G.M. O*Connor, T.J. Glynn, A.N. Volkov, and L.V. Zhigilei, Appl. Phys. A. 92, 791 (2008).

DS 5.4 Mon 16:30 H8

Thin films of $CoFe_2O_4$, ZnO, and $BaTiO_3$ patterned by micromoulding — •Ole F. Göbel, Tomasz Stawski, Sjoerd Veldhuis, Dave H.A. Blank, and Johan E. ten Elshof — Inorganic Materials Science, MESA+ Institute for Nanotechnology, University of Twente, the Netherlands

Thin films of functional oxides such as $CoFe_2O_4$, ZnO, or $BaTiO_3$ were derived from polymeric or sol-gel precursor solutions. Patterning the still liquid precursor films by simple micromoulding, followed by drying and pyrolysis, eventually yielded patterned oxide films, patterns having feature sizes of a few micrometer. The features, such as lines or dots, were completely isolated from each other. This low-cost technique requires very simple equipment and is applicable to a number of oxide material.

DS 5.5 Mon 16:45 H8

Diffuse Röntgenstreuung an Dünnschichtsystemen — •Malte Ernst, Dieter Lott, Wolfgang Kreuzpaintner und Andreas Schreyer — GKSS Research Centre Geesthacht, Germany

Diffuse Röntgenstreuung liefert wichtige Informationen über Grenzflächen von technologisch wichtigen Dünnschichtsystemen. Aus der diffusen Röntgenreflektivität lassen sich Größen wie Rauhigkeit, Korrelationslänge bzw Informationen über periodische Strukturen gewinnen. Dabei sind sowohl laterale wie auch vertikale Periodizitäten sichtbar. Zur Beschreibung der diffusen Streuung wird die *Distorted Wave Born Approximation* (DWBA) genutzt [1]. Dabei spielt im Dünnschichtsystem die Selbstkorrelation der einzelnen Grenzfläche und im Mehrschichtsystem auch die Kreuzkorrelation der einzelnen Grenzflächen eine wichtige Rolle. Mit Hilfe dieser Korrelationsfunktionen lässt sich unter Verwendung der DWBA der Strukturfaktor und somit die Streuintensität in Abhängigkeit des Impulsübertrages bestimmen. Die berechneten Reflektivitäten werden an realen Systemen getestet.
[1] S.K. Sinha et al., Phys.Rev.B 38, 2297 (1988)

DS 5.6 Mon 17:00 H8

High Temperature Interface Superconductivity — •Gennady Logvenov[1,2], Ivan Bozovic[2], and Adrian Gozar[2] — [1]Max-Planck-Institute for Solid State Research, Heisenbergstr.1, D-70569, Stuttgart — [2]Brookhaven National Laboratory, Upton, NY 11973,USA

Using atomic-layer molecular beam epitaxy we synthesize cuprate bilayers which show interface superconductivity. The superconducting critical temperature (T_c) in the bilayers structures depends on the deposition sequence: $T_c = 15\,\mathrm{K}$ in insulator-metal bilayers, while $T_c = 36\,\mathrm{K}$ in metal-insulator hetero-structures. In this talk I will present a comprehensive study of the high-temperature interface superconductivity, including transport measurements, crystal structure determination, and quantitative evaluation of Sr-La intermixing and of redistribution of mobile carriers across the interface. By a new technique, *delta-doping tomography* using isovalent Zn markers, we have demonstrated that in these heterostructures high-T_c superconductivity occurs within a single CuO_2 plane.

DS 6: [HL] Organic Semiconductors: Solar Cells (Joint Session DS/CPP/HL/O)

Time: Monday 16:00–17:45 Location: H15

DS 6.1 Mon 16:00 H15

Pulsed Photocurrent Measurements in Bulk Heterojunction Solar Cells — •Markus Mingebach[1], Moritz Limpinsel[1], Alexander Wagenpfahl[1], Alexander Goldmann[1], Carsten Deibel[1], and Vladimir Dyakonov[1,2] — [1]Experimental Physics VI, Physical Institute, Julius-Maximilians-University of Würzburg, Am Hubland, D-97074 Würzburg — [2]Centre of Applied Energy Research (ZAE Bayern e. V.), Am Hubland, D-97074 Würzburg

The performance of organic bulk heterojunction solar cells greatly improved during the last years up to 6% power conversion efficiency. Nevertheless very important properties such as the voltage dependent photocurrent are not fully understood yet. We investigate the photocurrent in poly(3-hexyl thiophene) (P3HT) : [6,6]-phenyl-C_{61} butyric acid methyl ester (PCBM) solar cells by applying a pulsed measurement technique (proposed by Ooi et al.) and also find a point of optimal symmetry (POS) at 0.52-0.64 V. In contrast to Ooi we identify this voltage not as the built-in voltage, but as the case of flat bands in the bulk of the cell (confirmed by macroscopic simulations). [1] To explain the voltage dependent photocurrent, we apply a combination of Onsager–Braun (polaron pair dissociation) and Sokel–Hughes (charge carrier extraction) theory in conjunction with the POS. In addition we observe and investigate a voltage-independent offset of the photocurrent, which is crucial for optimizing the device performance.
[1] M. Limpinsel, A. Wagenpfahl, M. Mingebach, C. Deibel and V. Dyakonov, Investigation of the Photocurrent in Bulk Heterojunction Solar Cells, submitted (2009).

DS 6.2 Mon 16:15 H15

Analytical analysis of the CELIV theory — •Jens Lorrmann[1], Bekele Homa Badada[2], Carsten Deibel[1], Olle Inganäs[2], and Vladimir Dyakonov[1,3] — [1]Experimental Physics VI, Physical Institute, Julius-Maximilians University of Würzburg — [2]Biomolecular and Organic Electronics, IFM, Linköping University, Sweden — [3]ZAE Bayern, Div. Functional Materials for Energy Technology, Würzburg

Charge extraction by linearly increasing voltage (CELIV) has attracted much interest in organic semiconductor research, due to its feature of measuring charge carrier mobility and density directly and simultaneously. Up to now the theoretical description of this method has been solved for a low mobility approximation only, because the general solution was impeded by a Ricatti type first order differential equation. In this contribution we present the analytical solution for this Ricatti equation, thus completing the analytical framework of the CELIV method. We compare it with the approximated theory and show that especially for standard organic solar cell materials the low mobility approach is hardly valid. The evaluation of photo-CELIV measurements on poly(3-hexyl thiophene-2,5-diyl):[6,6]-phenyl-C$_{61}$ butyric acid methyl ester solar cells can then be done by fitting the current transients. Surprisingly the fit results are only in a good agreement with the experimental currents, if two extraction currents are taken into account – the origin of which we will discuss. Furthermore we present a new equation for mobility evaluation from numerical analysis within our framework, which can be applied over the entire experimental range.

DS 6.3 Mon 16:30 H15

Oxygen Induced Degradation of P3HT:PCBM Solar Cells — •Julia Schafferhans, Stefan Neugebauer, Andreas Baumann, Alexander Wagenpfahl, Carsten Deibel, and Vladimir Dyakonov — Experimental Physics VI, Faculty of Physics and Astronomy, Julius-Maximilians-University of Würzburg, Am Hubland, 97074 Würzburg, Germany

Power conversion efficiencies of 6% for organic solar cells have already been achieved, with growing tendency. A critical issue yet to be addressed are the factors influencing the device lifetime. To gain a detailed understanding of the device stability, the underlying degradation mechanisms and their impact on the solar cell performance is an important prerequisite for lifetime enhancement. We investigated the oxygen induced degradation of state of the art (PCE $>$ 3%) P3HT:PCBM (poly(3-hexylthiophene):[6,6]-phenyl C61 butyric acid methyl ester) solar cells in the dark as well as under simultaneous illumination. Current–Voltage measurements are supplemented by Thermally Stimulated Current (TSC) and Charge Extraction by Linearly Increasing Voltage (CELIV) measurements. In the case of dark degradation the influence of oxygen results in a decrease of the short circuit current (Isc), whereas degradation under bias light leads to a decrease of all solar cell parameters. With the aid of a macroscopic simulation we demonstrate that the origin of the loss in Isc is oxygen doping, which we confirmed by CELIV measurements. In addition, TSC and CELIV measurements revealed an increase of deeper traps and a slight decrease of the mobility due to oxygen.

DS 6.4 Mon 16:45 H15

Polaron Recombination Dynamics in Bulk Heterojunction Solar Cells — •Andreas Baumann[1], Alexander Wagenpfahl[1], Carsten Deibel[1], and Vladimir Dyakonov[1,2] — [1]Experimental Physics VI, Physical Institute, Julius-Maximilians-University of Würzburg, Am Hubland, D-97074 Würzburg — [2]Centre of Applied Energy Research (ZAE Bayern e. V.), Am Hubland, D-97074 Würzburg

Organic solar cells with more than 6% power conversion efficiency were recently shown, coming closer to commercialization. For further improvements, a better understanding of the loss mechanisms inside the solar cell are needed, such as the recombination of photo-generated charge carriers. We applied the experimental technique of charge extraction by linearly increasing voltage (Photo-CELIV) to investigate the recombination dynamics in poly(3-hexylthiophene) (P3HT) : [6,6]-phenyl-C$_{61}$ butyric acid methyl ester (PCBM) bulk heterojunction solar cells. It was found experimentally, that the dominating polaron loss mechanism in P3HT:PCBM solar cells is of Langevin type, but reduced by a factor in the range of 0.1 in pristine samples to 0.01 in annealed ones [1]. We propose a model taking the charge carriers profile inside the active layer into account, which describes the origin of the observed reduced Langevin recombination [2].

[1] C. Deibel, A. Baumann, V. Dyakonov, APL 93, 252104 (2008)
[2] C. Deibel, A. Wagenpfahl, V. Dyakonov, PRB 80, 075203 (2009)

DS 6.5 Mon 17:00 H15

Relation of open circuit voltage to charge carrier concentration in organic bulk heterojunction solar cells — •Daniel Rauh[1], Alexander Wagenpfahl[2], Carsten Deibel[2], and Vladimir Dyakonov[1,2] — [1]Bavarian Centre for Applied Energy Research e.V. (ZAE Bayern), D-97074 Würzburg — [2]Julius-Maximilians-University of Würzburg, Institute of Physics, Experimental Physics VI, D-97074 Würzburg

A deeper understanding of the open circuit voltage V$_{oc}$ in bulk heterojunction solar cells is crucial for further performance enhancements. In order to investigate V_{oc}, we measured temperature dependent current–voltage characteristics of poly(3-hexylthiophene):[6,6]-phenyl C61 butyric acid methyl ester (P3HT:PCBM) solar cells (pristine and annealed) at various light intensities. With charge extraction measurements under the same conditions we could determine the corresponding charge carrier densities n in the operating device. Extrapolating V_{oc} to T=0K gives a constant value for all intensities indicating the effective bandgap of the donor–acceptor system. Fitting the data with V_{oc} models [1,2] showed excellent agreement with only one free parameter, the effective density of states. From our analysis, we gain insights into the recombination meachanisms limiting V_{oc}.

[1] Koster et al., Appl. Phys. Lett. 86, 123509 (2005)
[2] Cheyns et al., Phys. Rev. B 77, 165332 (2008)

DS 6.6 Mon 17:15 H15

Charge Carrier Concentration and Temperature Dependent Recombination in Polymer-Fullerene Solar Cells — •Alexander Foertig[1], Andreas Baumann[1], Daniel Rauh[2], Thiemo Gerbich[1], Vladimir Dyakonov[1,2], and Carsten Deibel[1] — [1]Experimental Physics VI, Physical Institute, Julius-Maximilians-University of Würzburg, Am Hubland, D-97074 Würzburg — [2]Centre for Applied Energy Research (ZAE Bayern e.V.), Am Hubland, D-97074 Würzburg, Germany

We performed temperature dependent transient photovoltage and photocurrent measurements on poly(3-hexyl thiophene):[6,6]-phenyl-C$_{61}$ butyric acid methyl ester bulk heterojunction solar cells. Thus we determined small perturbation carrier lifetime and charge carrier densities under operating conditions. We found a strongly charge carrier concentration and temperature dependent Langevin recombination prefactor. The observed recombination mechanism is discussed in terms of a bimolecular loss and compared with charge carrier extraction by linearly increasing voltage (photo-CELIV) measurements done on the same blend system. The observed charge carrier dynamics, following an apparent order larger than two, are explained by dynamic trapping of charges in the tail states of the Gaussian density of states.

DS 6.7 Mon 17:30 H15

Charge Carrier Generation Yield in Organic Solar Cells using a C80 Derivative as Acceptor — •Moritz Liedtke[1,2], Andreas Sperlich[2], Hannes Kraus[2], Andreas Baumann[2], Carsten Deibel[2], Vladimir Dyakonov[1,2], and Claudia Cardona[3] — [1]Centre for Applied Energy Research (ZAE Bayern e. V.), Am Hubland, D-97074 Würzburg, Germany — [2]Experimental Physics VI, Physical Institute, Julius-Maximilians-University of Würzburg, Am Hubland, D-97074 Würzburg — [3]Luna Innovations Incorporated, 521 Bridge Street, Danville, VA 24541 (USA)

Organic solar cells (OSC) with C$_{70}$ and C$_{80}$ fullerenes show a higher open circuit voltage (Voc) than the standard [6,6]-phenyl-C[61]-butyric acid methyl ester (PCBM):poly-3-hexylthiophene (P3HT) bulkheterojunction cells. Devices containing the trimetallic nitride endohedral fullerene Lu$_3$:N@C$_{80}$ showed a Voc of 910mV compared to 600mV with C$_{60}$-PCBM. Still the overall efficiency of these cells remain below the performance of our C$_{60}$-PCBM:P3HT reference cells. We address the origin of the lower efficiency by means of optical, magnetic and current measurement techniques. In samples containing Lu$_3$:N@C$_{80}$ we found photoluminescence quenching 3.2 times weaker, triplet yield higher and short-cut current about 2mA/cm^2 lower than in cells with C$_{60}$-PCBM as acceptor. We conclude that less efficient charge carrier generation in the Lu$_3$:N@C$_{80}$:P3HT bulkheterojunction system is the reason for the lower photocurrent.

DS 7: [MA] Multiferroics I (Joint Session of MA/DF/KR/DS)

Time: Monday 10:15–12:45 Location: H3

Invited Talk DS 7.1 Mon 10:15 H3

Antiferromagnetic interlayer coupling in $La_{0.7}Sr_{0.3}MnO_3$ / $SrRuO_3$ superlattices — •Ionela Vrejoiu — Max Planck Institute of Microstructure Physics, Halle, Germany

Perovskite oxides are versatile materials with a broad spectrum of physical properties, such as (anti)ferromagnetism, (anti)ferroelectricity, superconductivity, and multiferroicity. As illustrating examples, $La_{0.7}Sr_{0.3}MnO_3$ (LSMO) and $SrRuO_3$ (SRO) are both ferromagnetic perovskites with bulk ferromagnetic Curie temperatures of 370 K and 160 K, respectively. LSMO is a 3d transition metal double exchange ferromagnet, whereas SRO is a rare case of a 4d itinerant metallic ferromagnet and, in contrast to LSMO, SRO shows exceptionally strong magneto-crystalline anisotropy. Such differences make the interlayer coupling between LSMO and SRO epitaxial thin films an intriguing case. We report on LSMO / SRO superlattices (SLs) grown by pulsed-laser deposition on vicinal TiO_2-terminated $SrTiO_3$ (100) (STO) substrates. These SLs exhibit strong antiferromagnetic (AF) interlayer coupling at temperatures below 140 K, where the SRO layers become ferromagnetic. SLs in which an ultrathin nonmagnetic perovskite spacer was grown in between all the LSMO and SRO layers (so that the LSMO and SRO have no mutual interfaces) exhibited ferromagnetic coupling below 140 K. This indicates that the AF coupling occurs only in SLs with direct interfaces between LSMO and SRO. A joint study of structural characterization, SQUID magnetometry as well as first principles calculations was performed, in order to unravel the origin of this strong AF coupling.

DS 7.2 Mon 10:45 H3

Magnetic phase transition at a biferroic interface predicted from first principles — •Michael Fechner[1], Igor Maznichenko[2], Sergey Ostanin[1], Arthur Ernst[1], Jürgen Henk[1], and Ingrid Mertig[1,2] — [1]MPI für Mikrostrukturphysik Halle, Germany — [2]Fachgruppe Theoretische Physik, Martin-Luther-Universität Halle-Wittenberg

The interface magnetoelectric effect mediates the change of the magnetization at a ferromagnetic/ferroelectric interface when the electric polarization is modified. Using first principle methods, we investigate different ultrathin ferromagnetic films (Co and Fe) on top of ferroelectric $ATiO_3$ (A=Pb,Ba) perovskites upon the occurrence of it. The calculations show that at the interface a moderately change of the size of the total magnetization takes place [1]. Further the magnetic ordering of the Fe film is sensitive to its thickness, so an unexpected antiferrimagnetic ordering appears for 2ML Fe whereas for all other thicknesses ferromagnetic ordering is preferred. Hybridization and strain effects at the interface can explain all observations. An interesting perspective for further studies will be the investigation of thin films of a CoFe alloy. This may allow gaining control of the magnetic ordering by the electric polarization.

[1] Fechner et al.. PRB 78, 212406(2008)

DS 7.3 Mon 11:00 H3

Magnetoelectric coupling at modified Fe/$BaTiO_3$ interfaces — •Martin Hölzer[1], Michael Fechner[2], Sergey Ostanin[2], and Ingrid Mertig[1,2] — [1]Martin-Luther-Universität Halle-Wittenberg, Fachbereich Physik, D-06900 Halle, Germany — [2]Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle, Germany

Two-component multiferroics are gaining attention within the last years. These compound materials, consisting of ferromagnetic and ferroelectric layers, combine the advantages (e. g. high curie temperatures) of their components in a tuneable magnetoelectric structure.

Ab initio DFT studies of ultrathin Fe films on ferroelectric $BaTiO_3$ show that their magnetoelectric coupling can be enhanced considerably by means of interface alloying.

In these systems, the magnetoelectric coupling is related to structural changes in the interface region under polarisation reversal of the $BaTiO_3$ substrate. In one of the considered cases, a magnetic phase transition with high change in the total magnetization is triggered under polarization reversal.

DS 7.4 Mon 11:15 H3

Towards ferroelectric tunneling barriers with magnetic electrodes — •Daniel Pantel, Dietrich Hesse, and Marin Alexe — Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, 06120 Halle

The tunneling magnetoresistance (TMR) is a well-established quantum phenomenon in oxide electronics [1]. Recently, tunneling electroresistance was experimentally investigated in an oxide ferroelectric tunneling barrier [2, 3]. Combining both functionalities in one device, i.e. a ferroelectric barrier sandwiched in between two ferromagnetic electrodes, yields interesting properties, e.g. different effects of the ferroelectric polarization on the two spin channels [4]. However, experimental results are still lacking.

In this talk we report on the growth and the properties of perovskite oxide heterostructures consisting of a pulsed laser deposition-grown thin ferroelectric barrier layer sandwiched between two magnetic electrodes. First electrical measurements on capacitor-like tunneling junctions are presented.

[1] De Teresa, J.M., *et al.*, Science **286**, 507 (1999)
[2] Contreras, J.R., *et al.*, Appl. Phys. Lett. **83**, 4595 (2003)
[3] Garcia, V., *et al.*, Nature **460**, 81 (2009)
[4] Velev, J.P., *et al.*, J. Appl. Phys. **103**, 07A701 (2008)

DS 7.5 Mon 11:30 H3

Multiferroic materials with a non-collinear spin structure - A many-particle approach — •Thomas Michael[1], Julia M. Wesselinowa[2], and Steffen Trimper[1] — [1]Institute of Physics, Martin-Luther-Universität Halle-Wittenberg, Germany — [2]Department of Physics, University of Sofia, Sofia, Bulgaria

Multiferroic bulk materials with a conical spin structure are investigated in the framework of a many-particle approach. The analysis of the ferroelectric subsystem is based on a two-state quantum model. Magnetic moments interact via the Heisenberg model. The canting of the spins is incorporated by the Dzyaloshinski-Moriya interaction. A representation of the spin operators with an arbitrary quantization axis is chosen. Minimizing the free energy yields the direction of the quantization axis. The multiferroic coupling term is discussed. A Green's function technique in reciprocal space provides the temperature dependence of the magnetization, polarization and the energy of the excitations.

DS 7.6 Mon 11:45 H3

Manipulating ferroelectric domains of multiferroic $DyMnO_3$ by soft X-rays — •Victor Soltwisch, Enrico Schierle, Detlef Schmitz, Dimitri Argyriou, Fabiano Yokaichiya, Ralf Feyerherm, and Eugen Weschke — Helmholtz Zentrum Berlin

In multiferroic $DyMnO_3$, ferroelectricity is induced by cycloidal magnetic structures of a chirality coupled to the direction of the electric polarization. XRMS at the Dy-M5 resonance allows to distinguish surface regions of different chirality of the Dy-4f magnetic cycloid and, hence, can be used to image ferroelectric domains. Furthermore, the x-ray beam itself can be utilized to manipulate the distribution of domains at the crystal surface.

DS 7.7 Mon 12:00 H3

Evidence of electro-active excitation of the spin cycloid in $TbMnO_3$ — •Alexey Shuvaev[1], Viktor Travkin[2], Vsevolod Ivanov[2], Alexander Mukhin[2], and Andrei Pimenov[1] — [1]Experimentelle Physik 4, Universität Würzburg, D-97074 Würzburg, Germany — [2]General Physics Institute, Russian Academy of Science, 119991 Moscow, Russia

The coupling between the magnetic and ferroelectric orders in multiferroics is currently a topic of intense study. The materials of particular interest are those where the incommensurate cycloidal ordering of the spins drives the ferroelectricity. One of the consequences of multiferroicity is the existence of novel coupled magnon-phonon excitations called electromagnons. In addition to the electromagnon along the *a*-axis, the polarization analysis of the experimental spectra suggests the existence of an electro-active excitation for ac electric fields along the crystallographic *c*-axis. This excitation is possibly the electro-active eigenmode of the spin cycloid in $TbMnO_3$, which has been predicted within the inverse Dzyaloshinskii-Moriya mechanism of magnetoelectric coupling.

DS 7.8 Mon 12:15 H3

Neutron scattering studies on chiral multiferroics: magnetic structure and excitations — •T. Finger[1], M. Baum[1], A. C. Komarek[1], D. Senff[1], P. Link[6], K. Hradil[5], K. Schmalzl[4], W. Schmidt[4], L.-P. Regnault[3], D. N. Argyriou[7], P. Becker-Bohaty[2], L. Bohaty[2], and M. Braden[1] — [1]II. Physikalisches Institut, Universität zu Köln — [2]Institut für Kristallographie, Universität zu Köln — [3]CNG-Grenoble / ILL, Grenoble — [4]FZ Jülich, JCNS at ILL, Grenoble — [5]Universität Göttingen / FRM2 München — [6]FRM2, TU München, München — [7]HMI, Berlin

We present neutron-scattering experiments on IN12 and on IN14 using spherical polarization analysis directly documenting the poling of the elastic magnetic chiral terms for the spiral magnets MnWO$_4$ and TbMnO$_3$ by cooling in an electric field. In addition, we were able to observe a multiferroic hysteresis curve as function of electric field in both compounds and succeeded to switch the spiral at constant temperature, which is the central issue in view of future applications. Additionally, measurements of the diffuse scattering slightly above the multiferroic transition show some small chiral terms remaining in the collinear phase. The close coupling of ferroelectricity and magnetism in the multiferroic materials also results in new collective excitations, predicted almost 20 years ago: hybridised spin-phonon excitations, referred to as "electromagnons". After the first observations of potential electromagnon modes in infra-red and in neutron studies a conclusive interpretation is still missing. Our most recent neutron scattering measurements will be discussed.

DS 7.9 Mon 12:30 H3

Topological magnetoelectric memory effect in the spin-spiral multiferroic MnWO$_4$ — •Dennis Meier[1], Naemi Leo[1], Thomas Lottermoser[1], Petra Becker[2], Ladislav Bohatý[2], and Manfred Fiebig[1] — [1]HISKP, Universität Bonn — [2]Institut für Kristallographie, Universität zu Köln

Within the field of multiferroics, i.e. compounds with coexisting magnetic and electric order, so-called spin-spiral ferroelectrics attract tremendous attention. In these systems magnetic long-range order violates the inversion symmetry and induces a spontaneous electric polarization. Magnetic and electric domains are thus rigidly coupled so that “giant” magnetoelectric effects are obtained. However, up to now nearly nothing is know about the topology of the domain state in these systems. We report spatially-resolved measurements of the multiferroic domain topology in MnWO$_4$. For the first time, the full three-dimensional domain structure in a spin-spiral system is imaged. Our study reveals that the multiferroic domains in magnetically-induced ferroelectrics unify features that are associated to a magnetic domain state and others that point unambiguously to ferroelectric domains. Hence, a description in terms of ferroelectric or antiferromagnetic domains is incomplete and no longer appropriate. The novel concept of “multiferroic hybrid domains” is introduced. Annealing cycles reveal a topological memory effect: Due to phase coexistence at one phase boundary limiting the multiferroic state in MnWO$_4$, the entire multiferroic multidomain state can be reconstructed subsequent to quenching it. This work is supported by the DFG through SFB608.

DS 8: [MA] Multiferroics II (Joint Session of MA/DF/KR/DS)

Time: Monday 14:00–17:45 Location: H3

DS 8.1 Mon 14:00 H3

Switching of a spin-spiral-induced polarization in multiferroic MnWO$_4$ — •Tim Hoffmann[1], Dennis Meier[1], Petra Becker-Bohatý[2], Ladislav Bohatý[2], and Manfred Fiebig[1] — [1]HISKP, Universität Bonn — [2]Institut für Kristallographie, Universität zu Köln

Coexisting ferroic orders become interesting when there is an interaction between them. Especially applying an electric field and thus changing the magnetic order is highly desirable for possible applications. In spite of the declared interest in multiferroics to switch a magnetization by an electric field nothing is known about the dynamics of the actual switching process.

The coupling of ferroelectric and magnetic order is intrinsically strong in spin-spiral multiferroics, where ferroelectricity emerges as a consequence of complex magnetic long-range order. Here we observe the manipulation of magnetically-induced ferroelectric domains in MnWO$_4$ by optical second harmonic generation (SHG). Application of an electric field allows to transform the sample to an electric as well as magnetic single-domain state. Moreover we obtained images of the domain structures during the transition revealing the growth of the domains. When cooled in zero-field, the domains have a bubble-like topology. Interestingly, after recovery from a single domain state the shape changes to a stripe structure and the domain size is significantly increased. Effects of the shape and duration of the electric-field poling pulses are investigated. Furthermore, in contrast to typical ionic ferroelectrics the spontaneous polarization can be switched without fatigue – no defects or pinning effects constrain the movement of domain walls.

DS 8.2 Mon 14:15 H3

Single Crystal X-ray diffraction studies on multiferroic YMn$_{2-x}$Fe$_x$O$_5$ — •Sven Partzsch[1], Jochen Geck[1], Norman Leps[1], Roberto Kraus[1], Dmitr Souptel[1], Bernd Büchner[1], and Enrico Schierle[2] — [1]IFW Dresden — [2]Helmholz-Zentrum Berlin

Temperature dependent single crystal X-ray diffraction studies of YMn$_{2-x}$Fe$_x$O$_5$ are presented. Upon cooling, the undoped material (x=0) orders antiferromagnetically below $T_{\mathrm{N}} \approx 45\,\mathrm{K}$ and becomes multiferroic below $T_{CE} \approx 39\,\mathrm{K}$. This multiferroic phase is destabilized rapidly with increasing Fe-content and we address here the reasons for this dramatic effect. The crystallographic study implies that the doped Fe mainly occupies the square pyramidal coordinated Mn position instead the octahedral one, which shows that these lattice sites are crucial for the MF properties.

In order to further characterize the electronic ordering in the ferroelectric phase of the undoped samples, we also applied soft resonant X-ray diffraction, which clearly shows that the oxygen states play an important role as well.

DS 8.3 Mon 14:30 H3

Electronic structure and magnetism in YFeMnO$_5$ — •Torsten Weissbach[1], Tilmann Leisegang[2], Axel Lubk[2], Dirk C. Meyer[3], and Sibylle Gemming[4] — [1]Inst. f. Theoretische Physik, TU Bergakademie Freiberg — [2]Inst. f. Strukturphysik, TU Dresden — [3]Inst. f. Experimentelle Physik, TU Bergakademie Freiberg — [4]Inst. f. Ionenstrahlphysik u. Materialforschung, Forschungszentrum Dresden

YFeMnO$_5$ crystallizes in the structure type of the orthorhombic RMn$_2$O$_5$ class of oxides. These show a series of antiferromagnetic phases with propagation vectors (1/2-δ, 0, 1/4+ϵ) below $T_N \approx 45$ K. For several of these phases, magnetism coexists with ferroelectricity. In YFeMnO$_5$, only one commensurable ferrimagnetic phase was found below $T_N = 165$ K, and ferroelectricity is absent. We apply crystallographic and quantum chemical methods to compare the Fe-substituted and the mangenese-only compounds. Diffraction experiments show slight displacements of the atom sites with increasing Fe content. The largest effects are related to crystal-field repulsion acting on the local metal 3d orbitals. The interaction between the magnetic metal ions is studied using DFT calculations starting with a bias magnetization of the atoms.

DS 8.4 Mon 14:45 H3

***Ab initio* calculations of the magnetic properties of perovskites under deformation** — •Igor Maznichenko[1], Corina Etz[2], Arthur Ernst[2], Martin Lüders[3], Ingrid Mertig[1,2], Zdzislawa Szotek[3], and Walter Temmerman[3] — [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 — [3]Daresbury Laboratory, Daresbury, Warrington WA4 4AD, Cheshire, United Kingdom

Materials with perovskite and perovskite-like structures demonstrate a broad spectrum of physical properties. Colossal magnetoresistance, ferroelectricity, multiferroicity, superconductivity, charge ordering, metal-insulator transition, Jahn-Teller and other effects are observed in perovskites. These properties of the mentioned materials with the common formula ABO$_3$ are very sensitive to the type of the cations A and B. La$_{2/3}$Sr$_{1/3}$MnO$_3$ (LSMO) is a strongly correlated 3d transition metal oxide with a Curie temperature (T$_C$) above RT

(370 K). For other La/Sr ratios different types of antiferromagnetism are observed. Other perovskite, ruthenate $SrRuO_3$ (SRO) is a 4*d* ferromagnet with $T_C = 160$ K.

Here we perform *ab initio* calculations for LSMO and SRO in ideal cubic, tetragonally distorted, and different orthorhombic structures. We focus on magnetic order and Curie temperature of the above mentioned structures in the different structural phases.

DS 8.5 Mon 15:00 H3

Electric field induced magnetization switching in strained EuO — •Marjana Ležaić, Konstantin Rushchanskii, Frank Freimuth, and Stefan Blügel — Institut für Festkörperforschung and Institute for Advanced Simulation, Forschungszentrum Jülich, 52425 Jülich, Germany

EuO is one of the rare materials combining a semiconducting gap and ferromagnetic ordering. Due to this property, EuO was suggested as a spin-filter in magnetic tunnel junctions [1]. It was shown that its ordering temperature T_C of 69 K can be increased further by doping with Gd [2], or by a reduction of the lattice parameter [3]. Recently, it has also been shown that a spin-polarized 2-dimensional electron gas can be formed at the EuO/LaAlO3 interface [4]. The list of properties that are not only interesting from the point of view of basic research, but also indicate possible applications, does not end here. A newly discovered property, ferroelectricity in strained EuO [5] puts this material into the class of multiferroics with relatively high T_C. Employing *ab-initio* calculations, we demonstrate how the ferroelectric property can be exploited in EuO films under tensile strain in order to achieve electric control of the magnetization direction.

[1] T. Santos and J. S. Moodera, Phys. Rev. B **69**, 241203 (2004).
[2] R. Sutarto, *et al*, Phys. Rev. B **80**, 085308 (2009).
[3] N. J. C. Ingle and I. S. Elfimov, Phys. Rev. B **77**, 121202(R) (2008).
[4] Y. Wang, *et al*, Phys. Rev. B **79**, 212408 (2009).
[5] E. Bousquet, N. A. Spaldin, Ph. Ghosez, arXiv:0906.4235v1.

DS 8.6 Mon 15:15 H3

Ferroelectric properties of $BiFeO_3$ thin films under mechanical stress — •Martin Hoffmann, Oliver Mieth, and Lukas M. Eng — Institut für Angewandte Photophysik, Technische Universität Dresden, D-01062 Dresden

Since ferroelectric properties (polarization, coercive field, etc.) of thin films can differ dramatically from the corresponding bulk values due to lattice-mismatch-induced strain, the systematic investigation of the impact of mechanical stress on the nm-length-scale is an indispensable step towards the general understanding of ferroic thin film physics.

In the present study, 150-nm-thick multiferroic $BiFeO_3$ films grown on (001)-oriented $SrTiO_3$ substrates were inspected with piezoresponse force microscopy (PFM) towards their ferroelectric domain distribution and their local ferroelectric hysteresis behavior under both tensile and compressive stress.

The systematic variation of the externally applied mechanical stress by substrate bending allowed us to compensate or to enhance the strain effect, which can be quantified by monitoring the coercive field as a function of the bending angle.

DS 8.7 Mon 15:30 H3

Strain effects in spinel ferrite thin films from first principles calculations — •Daniel Fritsch and Claude Ederer — School of Physics, Trinity College Dublin, Ireland

We present density functional theory calculations of the structural and magnetic properties of the inverse spinel systems $CoFe_2O_4$ (CFO) and $NiFe_2O_4$ (NFO). Both are insulating magnets with high magnetic ordering temperatures and large saturation magnetization, which have been of particular interest over the past few years as building blocks of multiferroic heterostructures [1]. In order to effectively design the magneto-electric response of such multiferroic heterostructures, a clear picture of strain-induced changes in the magnetic properties of CFO and NFO is particularly important. Here we present results for the structural and magnetic properties of both CFO and NFO, with special emphasis on strain-induced changes in the magnetocrystalline anisotropy energy (MAE). Our results are representative for (001)-oriented thin films of CFO and NFO, grown on different lattice-mismatched substrates. We find a large and strongly strain-dependent MAE for CFO, and a significantly smaller but also strongly strain-dependent MAE for NFO. We discuss the influence of cation order within the inverse spinel structure and analyze the effect of different exchange correlation functionals on the structural and magnetic properties.

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

15 min. break

DS 8.8 Mon 16:00 H3

Mechanism of ferroelectric instabilities in non-d^0 perovskites: $LaCrO_3$ versus $CaMnO_3$ — Tim Harris, Roman Kovacik, and •Claude Ederer — School of Physics, Trinity College Dublin, Ireland

The incompatibility of partial *d* occupation on the perovskite *B*-site with the standard charge transfer mechanism for ferroelectricity has been a central paradigm in multiferroics research [1]. Nevertheless, it was recently shown by density functional theory calculations that $CaMnO_3$ exhibits a polar instability that even dominates over the octahedral tilting for slightly enlarged unit cell volume [2]. Here, we present similar calculations for $LaCrO_3$, which has the same d^3 *B*-site electron configuration as $CaMnO_3$. We show that $LaCrO_3$ exhibits a similar, albeit somewhat weaker, volume-dependent polar instability as $CaMnO_3$, but while the Born effective charge (BEC) for the Mn^{4+} cation in $CaMnO_3$ is highly anomalous, the BEC for Cr^{3+} in $LaCrO_3$ is only slightly enhanced. We decompose the BECs for both systems in contributions of individual Wannier functions to elucidate the different driving force behind the polar instability in these systems.

[1] N. A. Hill, J. Phys. Chem. B 104, 6694 (2000). [2] S. Bhattacharjee et al., Phys. Rev. Lett. 102, 117602 (2009).

DS 8.9 Mon 16:15 H3

Multiferroicity in $EuTiO_3$ and $Eu_{1-x}Ba_xTiO_3$: *ab initio* characterization of crystalline, magnetic and electronic structure — •Konstantin Z. Rushchanskii[1], Marjana Ležaić[1], and Nicola A. Spaldin[2] — [1]Institut für Festkörperforschung, Quanten-Theorie der Materialien, Forschungszentrum Jülich GmbH, 52425 Jülich, and JARA-FIT, Germany — [2]Materials Department, University of California, Santa Barbara, CA 93106-5050, USA

We report a systematic study of possible structural transitions in $EuTiO_3$ and ordered $Eu_{1-x}Ba_xTiO_3$ mixed compounds. We investigated phonon spectra of $EuTiO_3$ and found strong M- and R-point instabilities, indicating antiferrodistortive structural deformations. In the ordered $Eu_{0.5}Ba_{0.5}TiO_3$ compounds, the antiferrodistortive deformation is replaced by significant ferroelectric distortions, involving not only Ti, but also the magnetic Eu cation. We will discuss several scenarios of ferroelectric and antiferrodistortive transitions and their coupling with the magnetic structure. Corresponding changes in the phonon structure will be compared with available experimental data.

DS 8.10 Mon 16:30 H3

Electronic and magnetic properties of $LuFe_2O_4$ — •Karsten Kuepper[1], Michael Raekers[2], Christian Taubitz[2], Manuel Prinz[2], Christine Derks[2], Manfred Neumann[2], Andrei V. Postnikov[3], Frank M. F. de Groot[4], Cinthia Piamonteze[5], Dharmalingam Prabhakaran[6], and Stephen J. Blundell[6] — [1]Institut für Festkörperphysik, Universität Ulm, Albert-Einstein-Allee 11, D-89081 Ulm, Germany — [2]Fachbereich Physik, Universität Osnabrück, Barbarastr. 7, 49069 Osnabrück, Germany — [3]LPMD, Paul Verlaine University and Institute Jean Barriol, Metz, France — [4]Department of Inorganic Chemistry and Catalysis, Utrecht University, Sorbonnelaan 16, 3584 CA Utrecht, Netherlands — [5]Swiss Light Source, Paul Scherrer Institut, 5232 Villigen PSI, Switzerland — [6]Department of Physics, University of Oxford, Clarendon Laboratory, Parks Road, Oxford, OX1 3PU, United Kingdom

$LuFe_2O_4$ is a compound showing fascinating magneto electric coupling via charge ordering. Electronic and magnetic properties of the charge ordered phase of $LuFe_2O_4$ are investigated by means of x-ray spectroscopic and theoretical electronic structure approaches [1]. We identified the electronic states of the valence band by means of valence band XPS-, and XES-spectroscopies, and GGA+U first principles calculations. Moreover, by applying XMCD, we are able to identify the spin ground state of $LuFe_2O_4$ in the charge ordered phase to be a 2:1 ferrimagnetic configuration, ruling out a frustrated magnetic state.

[1] K. Kuepper et al., Phys. Rev. B, Rapid Commun., in press.

DS 8.11 Mon 16:45 H3

Influence of Fe-substitution in $LiNi_{(1-x)}Fe_xPO_4$ on the antiferromagnetic structure — •Elke Künzel[1], Anne Zimmermann[1], Jiying Li[2], David Vaknin[2], and Manfred Fiebig[1]

— [1]HISKP, Universität Bonn — [2]Ames Labatory and Department of Physics, Iowa States Univerity, Ames, USA

The LiMPO$_4$ system (M=Fe, Ni, Co, Mn) includes crystallographically isostructural compounds with antiferromagnetic (AFM) order differing in the spin direction only. Thus, the system offers the opportunity to study fundamental mechanisms of AFM 180° domain formation in a range of similar but not identical compounds. In spite of their structural similarity, drastic differences in the domain topology are observed by optical SHG. Domains in LiNiPO$_4$ form anisotropic platelets whereas in LiFePO$_4$ they are isotropic and amoeba-like. It is yet unclear whether this surprising behaviour is due to the properties of the nickel ion or to the spin direction which points along z in LiNiPO$_4$ and along y in LiFePO$_4$.

In order to clarify this, samples with different mixing ratios of nickel and iron were studied. The domain structure of LiNiPO$_4$ was found to become aboeba-like for an iron substitution of «50%. An anomalous temperature dependence of the AFM order parameter and indications for a spin structure different from that of the end compounds was observed.

DS 8.12 Mon 17:00 H3

Non-Resonant Magnetic X-ray Scattering on Rare-Earth Iron Borates RFe$_3$(BO$_3$)$_4$ — •Jorge E. Hamann-Borrero[1], Martin Philipp[1], Olga Kataeva[2], Martin von Zimmermann[3], Christian Hess[1], Ruediger Klingeler[1], Alexander Vasiliev[4], Leonard Bezmaternykh[5], and Bernd Buechner[1] — [1]IFW Dresden, 01171 Dresden, Germany — [2]A.E.Arbuzov Institute of Organic and Physical Chemistry of the Russian Academy of Sciences, Kazan, Russia — [3]HASYLAB at DESY, Hamburg, Germany. — [4]Low Temperature Physics department, Faculty of Physics, Moscow State University, Moscow, Russia. — [5]L.V Kirensky Institute of Physics, Russian Academy of Sciences, Krasnoyarsk, Russia.

Non-resonant magnetic XRD (NRMXRD) experiments with photon energy of 100keV where performed on selected compounds of the RFe$_3$(BO$_3$)$_4$ family as a function of temperature and applied magnetic field. The results show the existence of several unexpected diffraction features, in particular the presence of a magnetic super-lattice peak, and the appearance of two reflections that violate the diffraction conditions for the low temperature phase $P3_121$ of the iron borates. The magnetic nature of the former is concluded from analysing the scattering cross section at high energies and the magnetic structure of the different compounds. It is shown that the magnetic reflection reveals the magnetic properties of the material. For GdFe$_3$(BO$_3$)$_4$, values for the component of the spin moment perpendicular to the scattering plane ($S_\perp$) have been determined as well as the angle between the spin moment and the hexagonal basal plane.

DS 8.13 Mon 17:15 H3

Electronic structure, magnetic and dielectric properties of the edge-sharing copper-oxide chain compound NaCu2O2 — •Philippe Leininger[1], Martin Rahlenbeck[1], Markus Raichle[1], Britta Bohnenbuck[1], Andrey Malyuk[2], Chengtian Lin[1], Bernhard Keimer[1], Eugen Weschke[2], Enrico Schierle[2], Shinichiro Seki[3], Yoshi Tokura[3], and John Freeland[4] — [1]Max-Planck-Institut für Festkörperforschung, Heisenbergstr. 1, D-70569 Stuttgart, Germany — [2]Helmholtz-Zentrum Berlin für Materialien und Energie, D-12489 Berlin, Germany — [3]University of Tokyo, Dept. of Applied Physics, Bunkyo-ku, Tokyo 113-8656, Japan — [4]Advanced Photon Source, Argonne National Laboratory, Argonne, IL 60439, USA

We report an experimental study of NaCu2O2, a Mott insulator containing chains of edge-sharing CuO4 plaquettes, by polarized x-ray absorption spectroscopy (XAS), resonant magnetic x-ray scattering (RMXS), magnetic susceptibility, and pyroelectric current measurements. The XAS data show that the valence holes reside exclusively on the Cu2+ sites within the copper-oxide spin chains and populate a d-orbital polarized within the CuO4 plaquettes. Our results also demonstrate a new orbital selection rule for RMXS that is of general relevance for magnetic structure determinations by this technique. Dielectric property measurements reveal the absence of significant ferroelectric polarization below TN, which is in striking contrast to corresponding observations on the isostructural compound LiCu2O2. The results are discussed in the context of current theories of multiferroicity.

DS 8.14 Mon 17:30 H3

Magnetoelectric effect in diluted antiferromagnet PbFe$_{0.5}$Nb$_{0.5}$O$_3$ — •Vladimir Shvartsman[1], Pavel Borisov[2], Wolfgang Kleemann[2], and Antoni Kania[3] — [1]Institut für Materialwissenschaft, Fakultät für Ingenieurwissenschaften, Universität Duisburg-Essen, Essen, Germany — [2]Angewandte Physik, Fakultät für Physik, Universität Duisburg-Essen, Duisburg, Germany — [3]Institute of Physics, University of Silesia, Katowice, Poland

Multiferroics, i. e. materials where two primary ferroic order parameters of magnetic and electric nature coexist, are of significant scientific and practical interest nowadays. Especially attractive are the multiferroics with enhanced magnetoelectric (ME) properties, which relate changes of polarization/magnetization to external magnetic/electric fields, respectively. While the linear ME effect has strong symmetry requirements and is rare, higher order ME couplings are allowed in all multiferroics. We report on investigations of magnetic and ME properties of (001)-oriented PbFe$_{0.5}$Nb$_{0.5}$O$_3$ (PFN) single crystals in the temperature range 5-300 K. PFN is ferroelectric below 385 K and antiferromagnetic below the Néel temperature, T$_N$=154 K. Temperature dependences of the magnetization exhibit a step like anomaly at T$_N$ and a maximum on zero-field cooled curves at 8 K. Below T$_N$, the system manifests a spontaneous second order ME effect (electrobimagnetic effect), which reaches a peak value around 20 K. Moreover, after field cooling the linear ME effect has been observed, which disappears above 8 K. The nature of the low-temperature magnetic anomaly and the temperature dependences of the ME effects are discussed.

DS 9: Poster: Synthesis of Nanostructured Films by Self-organization, Thermoelectric Thin Films and Nanostructures, High-k and Low-k Dielectrics, Layer Deposition Processes, Layer Growth, Layer Properties, Application of Thin Films, Surface Modification, Hard and Superhard Coatings, Metal Layers

Time: Monday 15:00–17:30 Location: Poster D1

DS 9.1 Mon 15:00 Poster D1

Nanocomposite thin films prepared by co-sputtering and via deposition from a cluster source — •Tilo Peter[1], Sven Bornholdt[2], Matthias Wolter[2], Thomas Strunskus[1], Vladimir Zaporojtchenko[1], Holger Kersten[2], and Franz Faupel[1] — [1]Institute for Materials Science, Kiel, Germany — [2]Institute of Experimental and Applied Physics , Kiel, Germany

Nanocomposites consisting of metal clusters embedded in a dielectric thin film exhibit very interesting functional properties [1]. Relying on surface diffusion during co-deposition for generating clusters may cause problems since it depends not only on the deposited material but also on the substrate. To obtain clusters independent of the substrate and with tunable size, we use a self-built cluster source that creates clusters from magnetron sputtered metal atoms. In this process the plasma parameters are controlled via a helium/argon mix. Test materials were Ag, Au and Cu.

Samples prepared by co-deposition of plasma polymerized HMDSO and metal clusters are compared to samples prepared by co-sputtering of Ag and SiO2. In-situ characterization is done by visible/uv optical emission spectroscopy. XPS is used for chemical characterization, and HRTEM serves to measure the cluster size and density distribution. In addition, visible/ uv optical emission spectroscopy is used to investigate the optical properties and plasmonic resonance of the clusters.

[1] Deposition of nanocomposites by plasmas F. Faupel, et al.
Contributions to Plasma Physics (2007), 47(7), 537-544

DS 9.2 Mon 15:00 Poster D1

Spatially and time-resolved optical emission spectroscopy of mid-frequency pulsed PECVD — •Marcus Günther, Siegfried Peter, and Frank Richter — Institute of Physics, Chemnitz Univ.

of Technol., 09107 Chemnitz, Germany

Asymmetric bipolar pulsed plasma discharges in the mid-frequency (m.f.) range are of increasing interest for the deposition of *a*-C:H and *a*-SiCN:H films. This technique is attractive for industrial applications (large area coating) but less investigated yet. Moreover, using directly coupled m.f. power supply enables to choose the substrate bias voltage independent of other process parameters.

Optical emission spectroscopy (OES) is a method to characterize electrical discharges and learn about the excited species without affecting the discharge. In m.f. PECVD, the discharge frequency is lower than the plasma frequency of electrons and even ions, so that charged particles can follow changes of the electrical field. This periodical movement of charged species in the m.f. plasma is reflected in the spatially and time-resolved optical emission spectra. The deposition of *a*-C:H from acetylene (C_2H_2) or isobutylene (C_4H_8), and of *a*-SiCN:H from trimethylsilane(3MS) nitrogen argon mixtures in 100 kHz-pulsed discharges was analysed. As one result, above the powered electrode of the m.f. discharges no clear dark space was observed. The measured time behaviour of the plasma induced emission of individual species implies different excitation mechanisms.

DS 9.3 Mon 15:00 Poster D1

Optimizing the PECVD-process for low temperature growth of carbon nanotubes — •Kerstin Schneider[1], Michael Häffner[1], Boris Stamm[2], Monika Fleischer[1], Claus Burkhardt[2], Alfred Stett[2], and Dieter Kern[1] — [1]Institut für Angewandte Physik, Universität Tübingen — [2]Naturwissenschaftliches und Medizinisches Institut an der Universität Tübingen

Carbon nanotubes (CNTs) are typically grown at temperatures above 700 °C. However in the case of many electronic and life-science applications, temperature sensitive substrates require the use of growth processes at temperatures below 400 °C. In particular for the fabrication of CNT-microelectrodes on neuro-implants flexible, temperature sensitive substrates like artificial mica and polyimide have to be used. In order to grow vertically aligned CNTs at such low temperatures, we apply plasma enhanced chemical vapor deposition (PECVD)growth techniques using optimized PECVD parameters. Optimization of these parameters includes the variation of pressure, growth time, catalyst material, catalyst thickness, and gas mixture. Quantitative results of CNT length and quality as well as optimal growth parameters for growth processes below 400 °C will be presented.

DS 9.4 Mon 15:00 Poster D1

Formation mechanism of noble metal nanoparticles in reactively sputtered TiO_2 films — John Okumu[1], Dominik Köhl[2], Alexander Sprafke[2], •Hendrik Holzapfel[2], Gero von Plessen[2], and Matthias Wuttig[2] — [1]Department of Physics, Kenyatta University, P. O. Box 43844-00100, Nairobi, Kenya — [2]I. Physikalisches Institut (1A), RWTH Aachen University, D-52056 Aachen, Germany

Recently a simple preparation method has been developed to prepare Ag nanoparticles in a TiO_2 matrix [1,2]. In this scheme, silver nanoparticles are formed in a TiO_2 matrix first by sputtering a thin (d = 15nm) silver film sandwiched between two reactively sputtered TiO_2 layers (d = 30nm); this is followed by an annealing process. To determine the formation mechanism of noble metal nanoparticles in the TiO_2 matrix, we compare the behavior of Ag with that of two similar noble metals, gold and copper, by using x-ray diffraction, x-ray reflectance and optical spectroscopy. Despite the similarity of the three noble metals, we find that no Cu and Au nanoparticles are formed. This is in striking contrast to the behavior observed for Ag. The difference can be explained by a three step process, which involves oxidation of the Ag upon reactive sputter deposition of TiO_2, dissociation of the Ag oxide upon annealing and Ag aggregation to form nanoparticles. These processes do not occur at all in the case of Au, and are much slower in the case of Cu.

[1] J. Okumo *et al.*, J. Appl. Phys., **97**, 094305 (2005)

[2] C. Dahmen *et al.*, Appl. Phys. Lett., **88**, 011923 (2006)

DS 9.5 Mon 15:00 Poster D1

Inkjet printed organic layers on planar and microstructured flexible substrates for organic thin film devices — •Peter Lewer[1], Kerstin Schulze[1], Silvia Janietz[1], Felix Stelzl[2], Chegnui Bekeny[2], and Uli Würfel[2] — [1]Fraunhofer-Institute for Applied Polymer Research (IAP), Geiselbergstr. 69, 14476 Potsdam, Germany — [2]Fraunhofer-Institute for Solar Energy Systems (ISE), Heidenhofstr. 2, 79110 Freiburg, Germany

Inkjet printing of functional organic materials as deposition method holds the advantage for high throughput and low-cost production of organic electronic devices on flexible substrates in the future such as organic field effect transistors (OFETs) or organic solar cells (OSCs) [1,2]. In this context a three-dimensional electrode structure on a flexible substrate can be used for special application such as high voltage supply [3]. Therefore we investigate the inkjet printing process on these micro- or nanostructured PMMA-foils. The printing process was especially influenced by the capillary forces of the electrode structures. Here we show our results of the inkjet printing of semiconducting layers consisting of poly(3-hexylthiophene) (P3HT) in these three-dimensional structures. The preparation was done under ambient conditions and resulted in smooth layers as analysed with atomic force microscopy (AFM) and transmission electron microscopy (TEM).

[1] H. Sirringhaus, T. Kawase, R.H. Friend, T. Shimoda, M. Inbasekaran, W. Wu, and E.P. Woo, Science 2000, 290, 2123. [2] P. Calvert, Chemistry of Materials 2001, 13, 3299. [3] M. Niggemann, W. Graf, und A. Gombert, Advanced Materials 2008, 20, 4055.

DS 9.6 Mon 15:00 Poster D1

Structure formation at organic-inorganic interfaces — •Florian Szillat and Stefan G. Mayr — Leibniz-Institut fuer Oberflaechenmodifizierung, Translationszentrum fuer regenerative Medizin und Fakultaet fuer Physik und Geowissenschaften der Universitaet Leipzig, Permoserstrasse 15, 04318 Leipzig

Organic-inorganic interfaces have attracted significant scientific interest during the past decade - primarily due to their applications in the fields of organic semiconductors and biomaterials. Detailed experimental and theoretical understanding - in particular of the inorganic-organic interaction - is still lacking. To address these aspects we employ polycarbonate thin films on metal alloy substrates, while our focus lies on structure formation during organic film deposition. Our metal alloy surfaces are prepared on thermally oxidized silicon wafers by electron beam evaporation, while polybisphenol A polycarbonate thin films are deposited afterwards by thermal evaporation. Structure formation is characterized primarily with atomic force microscopy and interpreted within the concept of stochastic rate equations for film growth in the presence of interfaces [1]. Based on these concepts, conclusions on the interface interactions are drawn.

[1] C. Vree and S.G. Mayr, Applied Physics Letters 94 (2009) 093110

DS 9.7 Mon 15:00 Poster D1

Condensation of silicon monoxide on Si(111) studied by infrared spectroscopy for different substrate temperatures — Steffen Wetzel, •Markus Klevenz, and Annemarie Pucci — Kirchhoff-Institut für Physik der Universität Heidelberg, INF 227, 69120 Heidelberg

The growth of thermally evaporated silicon monoxide (SiO) on a Si(111) surface was studied in situ by infrared spectroscopy under ultra-high vacuum conditions. Within the first stage of film growth a large shift of the main vibrational band from 864 cm^{-1} to the bulk value of 984 cm^{-1} was observed (at 300K). This effect can be assigned to different Si-O bond lengths of Si-O-Si bridges nearby the Si surface in comparison to the bulk material and was successfully modelled with an SiO_x (0<x<1) interlayer. Measurements at various substrate temperatures also reveal a clear shift of the vibrational peak position; below 300 K to lower wave numbers with decreasing substrate temperature and above 300 K to higher wavenumbers with increasing substrate temperature, respectively. For higher temperatures disproportioning of SiO into Si and SiO_2 becomes important whereas for the very low temperatures only the bonding geometry should be important. Both effects will be discussed in detail.

DS 9.8 Mon 15:00 Poster D1

Self-assembly of CF-polymer films on SiO_2 (001) from first-principles calculations — •Oliver Böhm[1,2], Roman Leitsmann[1], Philipp Plänitz[1,2], Christian Radehaus[1], Michael Schreiber[2], and Matthias Schaller[3] — [1]GWT-TUD GmbH, Material Calculations, Chemnitz, Germany — [2]Institut für Physik, Technische Universität Chemnitz, 09107 Chemnitz — [3]Globalfoundries Dresden Module Two GmbH & Co. KG, Germany

Polymeric materials with a low dielectric constant(low-k) are essential to the interlayer dielectrics used for the next-generation integrated circuits. However, along with the introduction of these materials a bunch of processing challenges appears. For example the contamination pre-

vention of the material during wet and dry processing steps plays a key role in the fabrication process.
In this study we investigate the formation of thin CF-polymer films on ultra low-k (ULK) material surfaces during c-C_4F_8 plasma etching. In particular we use density functional theory (DFT) to study the adsorption process of different CF-polymers on SiO_2 (001) surfaces, which serves as a prototypical ULK system. For different C_nF_{2n+x} molecules the most stable adsorption sides and geometries and their impact on the electronic structure will be discussed in detail.

DS 9.9 Mon 15:00 Poster D1

Annealing of Silicon Nanopatterns — •Monika Fritzsche, Adrian Keller, Stefan Facsko, Kilian Lenz, and Jürgen Fassbender — Institute of Ion Beam Physics and Material Research, Forschungszentrum Dresden-Rossendorf, 01314 Dresden, Germany

The morphology of surfaces strongly influences optical, electrical, and magnetic properties of thin films. By changing the morphology it is possible to tailor the material properties. Oblique low energy ion beam sputtering produces periodic ripple structures with periodicities in the nanometer range. During sputtering the region near to the surface gets amorphous and some metal is deposited on the surface, i.e. Cu from the sample holder. These ripple patterns can be used as templates. By using amorphous ripples only polycrystalline films can be grown. These films have an morphology induced dipolar anisotropy. In order to grow the films epitaxially the ripples have to be crystalline. Hence, this could induce an additional anisotropy in a magnetic overlayer. One possible route to achieve crystalline ripples is annealing. Therefore, the annealing temperature dependence was studied using STM. With increasing temperature the ripples vanish. They are not removed by a reduction of the amplitude, but by the creation of circular voids. Inside these voids the surface exhibits few steps and is otherwise flat on an atomic scale. In the middle of the voids Cu clusters are found, which appear at steps. Inside the crystalline area of the voids the Si(111) "quasi 5×5" Cu surface is found. For larger temperatures the number and size of these voids increases until the ripples are removed from the whole surface.

DS 9.10 Mon 15:00 Poster D1

Multiscale nanostructuring of Si surfaces combining top-down and bottom-up techniques — •Bashkim Ziberi, Frank Frost, Klaus Zimmer, and Bernd Rauschenbach — Leibniz-Institut ür Oberflächenmodifizierung (IOM), Permoserstrasse 15, D-04318 Leipzig, Germany

Surface patterning is of tremendous importance in many technological fields with features sizes ranging from nanometers to millimeters. There are different patterning techniques that generally can be assigned to the top-down and bottom-up approaches. One bottom-up method for the generation of self-organized nanostructures is low-energy ion beam erosion. However due to the stochasticity of the process there is a lack of large scale ordering of nanostructures and of positional control. Here results on self-organized nanostructuring of pre-patterned Si surfaces will be presented. The idea is to combine the top-down technique for pre-patterning of surfaces followed by the ion beam induced self-organization process. Due to the periodicity, shape and lateral ordering of pre-patterns an improved ordering, and an exact positional control of nanostructures is achieved. The method allows also for the formation of new structures and patterning of more complex surfaces like curved one or more difficult geometries are possible. The pre-patterned substrates are fabricated by various lithographic techniques in combination with etching techniques for structure transfer. Depending on the shape of the pre-patterned structure different results are obtained. Furthermore, using the imprint technique inverse pre-patterns (e. g. pits-holes) are used to study the self-organization process.

DS 9.11 Mon 15:00 Poster D1

Smoothening and patterning of Si surfaces produced by metal surfactant sputtering — •Kun Zhang and Hans Hofsäss — II. Physikalisches Institut, Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen

Surfactant sputtering provides a novel, versatile sputter technique utilizing the steady state coverage of a substrate surface with up to 10^{16} /cm^2 of foreign or self atoms simultaneously during sputter erosion by combined ion irradiation and atom deposition. Depending on the chemical relation of the materials between the substrate and the surfactant, nanocluster, nano-meter thin film or nano-compound can form on the substrate surface or be burred in the top layers of substrate, which strongly modify the substrate sputter yield on atomic to macroscopic length scales, and further more, produce different surface morphologies (smoothening or nano-pattern from dots to ripple). In this study, metal surfactants (such as Au, Ag, Pt, Ni, Fe and steel etc.) were used to produce ultra-smooth surface or different surface nano-pattern on silicon, specially at the incident angle near substrate normal direction, at which no nano-pattern would form in the absence of deposition of surfactant atoms, predicted by the Bradley-Harper theory and demonstrated by many experiments. Si(100) substrates were eroded using 5 keV Xe-ions at the fluence of up to 10^{18} /cm^2 under continuous deposition of metal atoms from surfactant targets, which were sputtered simultaneously by the same ion-beam. The surface topography, the composition, and the microstructure of the nanocomposites have been analyzed via RBS, AFM and TEM.

DS 9.12 Mon 15:00 Poster D1

Electrodeposition of ZnO for dye-sensitized cells on corrosion-resistive metal wires — •Kerstin Strauch, Melanie Rudolph, Thomas Loewenstein, and Derck Schlettwein — Institute of Applied Physics, Justus-Liebig-University Giessen, Germany. email:schlettwein@uni-giessen.de

This work is part of an initiative to develop a textile-based photovoltaic cell using the concept of dye-sensitization. For this purpose porous ZnO is deposited by electrodeposition and subsequently sensitized by an organic dye. The porous sensitized semiconductor electrode has to satisfy two conditions: First the substrate material has to be conductive and inert with the iodine containing electrolyte. Secondly the deposition of porous zinc oxide on the conductive textile or wire has to be homogenous and continuous. In this work different metal wires which had proven to be stable in the redox electrolyte were used as substrate electrodes. The conditions of electrodeposition were optimized for each of the metals. We either used a constant potential ("potentiostatic") mode in contact to an oxygen saturated $ZnCl_2$ solution or a pulsed deposition using the reduction of nitrate in a $Zn(NO_3)_2$ solution. The deposition process was monitored by the developed current under the given conditions. The obtained films were analyzed by confocal laser microscopy and scanning electron microscopy. The films were tested for their uptake of sensitizing dyes. The properties of the obtained electrodes in dye- sensitized solar cells will be discussed.

DS 9.13 Mon 15:00 Poster D1

Texturing of ZnO films on glass for use as a light-scattering layer in micromorphous silicon thin film solar cells — •Kambulakwao Chakanga — EWE-Forschungszentrum für Energietechnologie e.V., Next-Energy, Oldenburg, Germany

Light Trapping is a profound tool for enhancing solar cell efficiency by increasing light absorption and decreasing reflection. Glass/TCO interfaces with textured TCO layers are commonly implemented in micromorph solar cells to scatter incident light and increase the optical path. However altering the morphology of the front contact TCO also affects the optical and electrical properties of the solar cell.

This master thesis aims to analyse this relationship between the texture and the optoelectronic properties in ZnO:Al. ZnO:Al has been chosen because it is frequently argued as being more beneficial in comparison to commercially available TCOs. The commercially available ASAHI-U-type SnO2:F is analysed as a reference.

The different surface textures are obtained by wet chemical etching with different acids in different concentrations, at different etching periods. Subsequently the morphology is investigated by atomic force microscopy. The optical properties are measured by spectrometry. The haze factor is determined as a descriptive scatter parameter. Finally the electrical properties are measured with a Four-Point-Probe.

DS 9.14 Mon 15:00 Poster D1

Proton Beam Writing — •Martina Schulte-Borchers, Ulrich Vetter, and Hans Hofsäss — II. Physikalisches Institut, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, D-37077 Göttingen, Germany

Proton Beam Writing (PBW) is a direct-write lithography process for microfabrication of two- or three-dimensional structures. It can be used to manufacture microfluidic channels, wave guides, biosensors and other devices. Due to the maskless writing technique and the high spatial resolution obtained by the usage of protons, this method allows for the fabrication of structures with high aspect ratio and small structure width. This makes PBW preferable to other lithographic techniques like electron beam- or photolithography. We will describe the newly installed PBW system at the Goettingen 3MV Pelletron accelerator and discuss its technical characteristics together with first proton beam written structures.

DS 9.15 Mon 15:00 Poster D1

Correlation between Ion Bombardment, Lattice Expansion and Nitrogen Content After Nitriding of Austenitic Stainless Steel — •Darina Manova, Jürgen W. Gerlach, Stephan Mändl, and Horst Neumann — Leibniz-Institut für Oberflächenmodifizierung, 04318 Leipzig, Germany

Broadbeam low energy ion implantation is a versatile method for nitrogen insertion in transition metals containing alloys like austenitic stainless steel. The process is characterized by an anomalous high diffusivity leading to nitrogen enriched layers of up to several micrometers thickness coupled with an anisotropic lattice expansion of up to 12%. By using a radiation heater in addition to ion beam heating to maintain the process temperature between 350 and 450 °C, controlled continuously by pyrometer, and an electronic nitrogen ion beam switch, a reduced nitrogen ion flux was realised. As a result, the XRD peak widths of the resulting expanded austenite were reduced from about 2° to 0.7 * 0.9°, while a strong nitrogen concentration gradient was still observed within the first micrometers. Thus, the initial broadening is less related with a range of different nitrogen concentration dependent lattice expansions through the layer. At the same time, no linear correlation between the lattice expansion and the nitrogen content was observed, invalidating the use of Vegard*s law to estimate the nitrogen content from the lattice expansion.

DS 9.16 Mon 15:00 Poster D1

XPS Analysis of Phase Formation after Nitrogen Insertion in CoCr and FeCrNi Alloys — •Johanna Lutz[1,2], Jürgen W. Gerlach[1], and Stephan Mändl[1] — [1]Leibniz Institute of Surface Modification, Leipzig, Germany — [2]Translational Centre for Regenerative Medicine, University of Leipzig, Germany

Plasma immersion ion implantation for inserting nitrogen in transition metals like CoCr alloys or FeCrNi alloys is characterized by near surface ion implantation and a subsequently anomalous high diffusivity leading to nitrogen enriched layers up to several micrometers. At the same time, a lattice expansion of the original fcc structure by 5 to 10% is observed. Preferential trapping with the formation of Cr-N bonds inside the austenitic structure is acclaimed to explain the anomalous concentration profiles at lower temperatures, while beyond 450 °C a transition from the expanded austenite towards CrN precipitates occurs.

In this presentation, photo electron spectra (XPS) are investigated after nitrogen PIII in face-centred-cubic CoCr and FeCrNi alloys in the temperature range from 230 - 580 °C. The process was carried out at pulse voltages of -10 kV, a base pressure of 0.5 Pa and process time of two hours. For FeCrNi alloys, evidence of the nitrogen insertion is only found for the Cr2p peak, however independent of the process temperature, with no changes in the Fe2p and Ni2p core level spectra. For CoCr alloys, despite similar nitrogen concentrations of 30 to 35 at.%, no variation in either Co2p, Cr2p, Fe2p or Ni2p spectra was observed.

DS 9.17 Mon 15:00 Poster D1

Electrical properties of phase change materials along the pseudo binary line between GeTe and SnTe analysed with temperature dependent Hall effect measurements — •Felix Lange, Hanno Volker, Carl Schlockermann, Jenni Karvonen, and Matthias Wuttig — RWTH Aachen University, I. Physikalisches Institut (IA), 52056 Aachen, Germany

Phase change materials are a class of materials that can be reversibly switched between an amorphous and a crystalline state. These two states exhibit characteristic differences in their physical properties such as the reflectivity and the electrical resistivity. By assigning these two states to the binary values 1 and 0 one can store information as already realized in optical data storage media like CD±RW and DVD±RW. The electrical induced switching within nanoseconds [1] makes PC- materials also interesting for non-volatile RAM applications. It is obvious that a comprehensive understanding of the electrical transport properties is crucial in order to match the low power requirements of the device. Therefore we have investigated electrical properties along the pseudo binary line between GeTe and SnTe by temperature dependent Hall effect measurements.

[1] G. Bruns *et al.* (2009). App. Phys. Lett. **95**, 043108

DS 9.18 Mon 15:00 Poster D1

Field effect in GeTe thin films — •Hanno Volker, Carl Schlockermann, Daniel Krebs, Jörn Riedel, and Matthias Wuttig — RWTH Aachen University, I. Physikalisches Institut (IA), 52056 Aachen, Germany

Phase change memory is a promising candidate to replace common memory technologies such as Flash and DRAM due to its fast switching and excellent scaling perspectives. To improve memory density even further, it was proposed to combine the switchable resistor and the cell selection transistor in a single device. Current control by applying gate voltages has been demonstrated in the works of Yin et al. for $Ge_2Sb_2Te_5$ [1].

Recently, switching within a few nanoseconds has been demonstrated on a different material, GeTe [2]. We therefore studied the field effect in thin films of amorphous GeTe. Dedicated transistor devices were prepared, and the transfer characteristics of these devices were measured as a function of temperature and film thickness. Furthermore, time-dependent behavior was observed and analyzed.

[1] Y. Yin *et al.* (2006). *Japan. J. Appl. Phys.* **45**, 3238
[2] G. Bruns *et al.* (2009). *App. Phys. Lett.* **95**, 043108

DS 9.19 Mon 15:00 Poster D1

Investigation of the electrical properties of lithographically structured gold wires — •Kathrin Krüger, Peter Jost, Carl Schlockermann, Philipp Merkelbach, Karl Simon Siegert, and Matthias Wuttig — RWTH Aachen University, I. Physikalisches Institut (IA), 52056 Aachen, Germany

Ongoing miniaturization in electrical devices focuses the attention on thin film effects. Over the last decade, lithographic structures became continuously smaller. Thus, new demands are placed on the interconnects, which are realized by thin and small wires.

Because of its high conductivity and thermal stability at temperatures around room temperature, gold is an important candidate as contacting material. Gold wires are often applied to the substrate by evaporation, whereas glass or silicon is often used as substrate material. To obtain a better adhesion of the gold on glass substrates, a chromium adhesion layer can be used.

Therefore, for many measurements it is important to know the electrical properties of gold. However, it is not clear whether the electrical properties, such as the specific resistance and its temperature coefficient, are still close to bulk properties at small feature sizes. Thus, in this study the dependencies of the specific resistance and its temperature coefficient of lithographically structured and thermally evaporated gold wires on thickness and width are investigated. Also, it is studied how a chromium adhesion layer affects these electrical properties.

DS 9.20 Mon 15:00 Poster D1

The influence of Sb clusters on electrical characteristics in organic-semiconductor structures — •Markus Arnold[1], Yue Huang[2], Axel Fechner[1], and Dietrich R. T. Zahn[1] — [1]Chemnitz University of Technology, Semiconductor Physics, 09107 Chemnitz, Germany — [2]Fudan University, Department of Microelectronics, Shanghai 200433, China

Electrical characterization using capacitance-voltage (CV) and charge transient spectroscopy (QTS) of Al/copper phthalocyanine (CuPc)/Si structures are presented. The CuPc layer was modified by the incorporation of Sb clusters. In this case the CV-measurements reveal some hysteresis in contrast to structures without Sb. This is assigned to a charge trapping in the Sb clusters. In order to analyze this in detail QTS is applied.

QTS originally developed by Kirov *et al.* [1] is an electrical measurement technique related to deep-level transient spectroscopy (DLTS) developed by Lang *et al.* [2]. Using QTS it is possible to measure charge reloading processes even in the absence of a depletion region as a function of time and temperature with different pulse voltages and widths. As a result, one can determine the energetic position, the capture cross section, and the density of the electrically active traps.

[1] K. I. Kirov, K.B. Radev, Phys. Stat. Sol. (a) 63 (1981) 711
[2] D. V. Lang, J. Appl. Phys. 45 (1974) 3023

DS 9.21 Mon 15:00 Poster D1

Surface Enhanced Raman Effect of Silver Nanoparticle Covered Substrates Prepared by Nanosphere Lithography — •Michael Ludemann[1], Philipp Schäfer[1], Christoph Brombacher[2], Ovidiu Gordan[1], Manfred Albrecht[2], and Dietrich R. T. Zahn[1] — [1]Semiconductor Physics, Chemnitz University of Technology — [2]Surface and Interface Physics, Chemnitz University of Technology

Weak Raman signals can be strongly enhanced using the so called surface enhanced Raman scattering (SERS) effect employing *e.g.* nanostructured metal surfaces. In order to get a deeper understanding of the enhancement mechanisms, silver nanoparticles of well defined shape and size prepared by nanosphere lithography were applied instead of randomly roughened silver films. The dependence of SERS spectra of copper phthalocyanine (CuPc) on the film thickness is discussed. For this purpose monitoring of the Raman signal during deposition of the organic film was performed *in situ.*

DS 9.22 Mon 15:00 Poster D1

Electrical Resistivity and Hydrogen Solubility of PdHc Thin Films — •Stefan Wagner and Astrid Pundt — IMP, Uni Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen

Resistivity measurements are a commonly applied operator for the determination of pressure-concentration-isotherms in metal-hydrogen systems. Lee et al. [1] report on an anomalous reduction of the hydrogen induced resistivity change in PdHc thin films during hydrogen loading. Thermodynamic properties of thin films, respectivey, have been shown to be strongly interfered by microstructural and mechanical stress, appearing from thin film proprties such as nanostructure, clamping to a rigid substrate, related biaxial stress, the formation of microstructural defects and buckling. Therefore the question appears, whether there is a direct stress impact on the resistivity in PdHc thin films as well. Here we show [2] that the reduced resistivity response of PdHc thin films can mainly be attributed to a stress dependent reduction of the hydrogen solubility.

[1] Lee, M., Glosser, R.: Z. Phys. Chem., Neue Folge 147 (1986) 27. [2] Wagner, S., Pundt, A.: Acta Materialia (2009), doi:10.1016/j.actamat.2009.10.045

DS 9.23 Mon 15:00 Poster D1

Conducting ion track in tetrahedral amorphous carbon films — •Hans-Gregor Gehrke[1], Anne-Katrin Nix[1], Johann Krauser[2], Christina Trautmann[3], Alois Weidinger[4], and Hans Hofsäss[1] — [1]II. Physikalisches Institut, Universität Göttingen, Germany — [2]Hochschule Harz, Wernigerode, Germany — [3]Gesellschaft für Schwerionenforschung, Darmstadt, Germany — [4]Hahn-Meitner-Institut, Berlin, Germany

Swift heavy ions passing through insulating tetrahedral amorphous carbon (ta-C) films leave conducting tracks along their path. The huge energy loss of over 40 keV/nm of each ion transforms the ta-C with 80% sp^3 bonds into a graphite-like sp^2-rich phase creating nanosized filaments with a diameter of about 8 nm. The film thickness may vary from a few nanometers to micrometers allowing a vast range of aspect ratios. In addition, it is possible to interrupt the filaments with thin insulating layers which do not alter their conductivity during the irradiation process. This technique, allows the creation of embedded electrical quantum dot structures with dimensions in the nanometer regime. The dimensions are sufficiently small to achieve coulomb blockade effects even at room temperature. We analyzed the conduction of ion tracks and dot structures with different insulator thicknesses electrically on filament ensembles by macroscopic contact pads and single tracks measurements by AFM probing with a conducting tip.

DS 9.24 Mon 15:00 Poster D1

A novel setup for thermopower measurements on thin films — •Peter Jost, Carl Schlockermann, and Matthias Wuttig — RWTH Aachen University, I. Physikalisches Institut, 52056 Aachen, Germany

Thermopower measurements are a common mean to gain insight into the electrical transport phenomena of metals and semiconductors. The typical method relies on making electrical contacts to the sample with two thermocouples. By measuring the voltages between the legs of the two thermocouples the temperature difference between the thermocouples' junctions and the thermoelectric voltage drop on the surface of the sample can be obtained. However, this technique is limited to moderate resistive samples as the measurement amplifiers have to meet the conflicting requirements of the low resistive thermocouples and the high resistive samples at the same time.

We have developed a novel setup that allows thermopower measurements on high resistive thin film samples. By setting the temperatures of both ends of the substrate to the temperatures of the underling copper blocks electrical contacts and temperature measurement can be decoupled. Thus, the amplifiers can be matched purely to the impedance of the sample. Furthermore this technique allows the deposition of an electrically isolating capping layer on top of the film of interest.

In this work we explain our setup and show the advantages and limitations of our method.

DS 9.25 Mon 15:00 Poster D1

Electrical and thermal conductivity of individual cylindric nickel nanowires — •Johannes Kimling and Kornelius Nielsch — Institute of Applied Physics, University of Hamburg, Jungiusstr. 11, 20355 Hamburg

Thermoelectric nanowires (NWs) are predicted to exhibit a higher figure of merit ZT than the according bulk materials. In order to investigate the underlying physical mechanisms, measurements on individual NWs have to be realized. However due to the small length scales, electrical and thermal measurements in particular are challenging. Here, we report on measurements of the electrical and thermal conductivity of individual cylindric Ni NWs by means of 4-point measurements and by using the "3-omega self-heating" method, respectively.

Cylindric NWs of diameters between 20 nm and 400 nm are synthesized by potentiostatic electrodeposition of Ni in highly ordered alumina membranes. Before electrodeposition the pore channels of the templates were coated with silicon dioxide by means of atomic layer deposition. The silicon dioxide layer remains as a shell stabilizing the NWs after dissolution from the template.

For contact definition we use photolithography. Low contact resistances are achieved by controlled sputter etching to remove the oxide layer directly before the metallization of the electrodes. First results of a Ni NW with a radius of 180 nm show that the thermal conductivity and the Lorenz number are well below the bulk values.

DS 9.26 Mon 15:00 Poster D1

Thermal characterization of $ZnS:SiO_2$ — •Karl Simon Siegert, Carl Schlockermann, Philipp Merkelbach, Hanno Volker, and Matthias Wuttig — RWTH Aachen University, I. Physikalisches Institut (IA), 52056 Aachen, Germany

Phase change materials such as $Ge_2Sb_2Te_5$ or GeTe offer unique physical characteristics. Their strong changes in optical and electrical properties during their amorphous-crystalline phase transitions make them especially interesting for data storage applications [1]. The large contrast in reflectance between the amorphous and the fcc-phase of $Ge_2Sb_2Te_5$ is already technologically exploited in rewritable optical storage discs. As the switching between the amorphous and the crystalline state is induced by temperature, thermal characterization of the phase change material and all other surrounding materials is needed for further improvement of data storage devices. This work focuses on thin films of $ZnS:SiO_2$, a material, which is used for protective layers on top of the active phase change layer in optical storage media. We have created several samples of different thicknesses by sputter deposition and characterized them using AFM and XRR. Small gold wires were created on top of the sample by photo-lithography and were used to measure the cross-plane thermal conductivity with an AC-measurement technique.

[1] Wuttig *et al.* Nat. Mat. **6**, 824 - 832 (2007)

DS 9.27 Mon 15:00 Poster D1

Optical analysis of $ZnS:SiO_2$ used as a Capping layer for phase change alloys — •Stephanie Grothe, Peter Jost, Michael Woda, Jenni Karvonen, and Matthias Wuttig — RWTH Aachen University, I. Physikalisches Institut (IA), 52056 Aachen, Germany

Phase change materials which can be switched rapidly between the amorphous and the crystalline phase are a promising candidate for new memory devices. These materials can be identified by a strong contrast in the optical dielectric constant between both phases which is due to resonant bonding [1]. As the optical dielectric constant can be evaluated from the dielectric function it is of great importance to measure the dielectric function with high accuracy.

However, an exact investigation of the dielectric constant is impeded by ageing effects which occur in the alloys after sputtering. First, we explored the dielectric function of $Ge_1Sb_2Te_4$ by infrared spectroscopy and spectroscopic ellipsometry and analysed the effect of ageing on the optical spectra.

Then, we investigate how these ageing effects can be prevented by the use of a suitable capping layer. We found out that a thin layer of $ZnS:SiO_2$ sputtered on top of the phase change material prevents ageing to a large extend. Additionally, after taking the $ZnS:SiO_2$ surface layer into account we can still investigate the optical properties of phase change materials which are capped by $ZnS:SiO_2$.

[1] Shportko, K. *et al.*, *Nature Mater.* **7**, 653-658 (2008).

DS 9.28 Mon 15:00 Poster D1

Sb doped SnO2: attractive alternative TCO material for ITO — •Janika Boltz, Dominik Koehl, and Matthias Wuttig — I. Physikalisches Institut (IA) RWTH Aachen 52056 Aachen Germany

Transparent Conducting Oxides (TCO) are widely employed in applications such as displays, solar cells or architectural glazing. Most commonly used materials today are based on Indium Tin Oxide (ITO). Limited amounts of explorable Indium will soon lead to a shortage of ITO, thus alternatives based on other materials are needed. Sb-doped SnO2 films possess a high optical transparency and good electrical conduction, which makes them attractive for TCO applications. In order to deposit suitable films on large area substrates we have explored the properties of Sb-doped SnO2 thin films that have been prepared by reactive dc magnetron sputtering from a metallic target at room temperature. The films were subsequently analysed regarding their optical, electrical and structural properties. Our results show that there is only a narrow process window for the sputter deposition of transparent and conducting tin oxide films at room temperature. A sharp minimum in resistivity is observed at an oxygen content of approximately 17 % in the sputtering gas. Under these deposition conditions, the SnO2:Sb films turn out to be highly transparent and crystalline.

DS 9.29 Mon 15:00 Poster D1

Spectroscopic Characterisation of Amorphous Silicon Thin Films — •Philipp Schäfer[1], Frank Nobis[2], Hartmut Kupfer[2], Frank Richter[2], and Dietrich R. T. Zahn[1] — [1]Semiconductor Physics, Chemnitz University of Technology — [2]Solid State Physics, Chemnitz University of Technology

Amorphous Silicon (a-Si) and especially hydrogenated amorphous silicon is widely used in photovoltaic applications. Despite its lower total efficiency compared to crystalline silicon, a-Si has the advantage of cheaper and easier proccessing. It can be deposited at low temperatures, it is mechanically flexible, and it provides technically relevant films already at sub-micrometre film thicknesses. However, an elaborated understanding of the film properties is required in order to improve the preparation parameters.

In this work d.c.-pulsed magnetron sputtered a-Si films are probed with various spectroscopic techniques. Thus, a comprehensive picture of their properties is achieved: *Raman* spectroscopy provides access to the morphological aspects of the film. One can distinguish between microcrystalline, crystalline, and amorphous films. Furthermore, it allows a detailed morphological characterisation of amorphous film in terms of the spread in mean bond angle $\Delta\theta$ to be obtained. Fourier transform infrared spectroscopy, on the other hand, reveals the concentration of hydrogen. Variable angle spectroscopic ellipsometry is applied and the complex dielectric function $\varepsilon(\nu)$ of the a-Si layer is evaluated using a *Tauc-Lorentz* model. A detailed comparison of a-Si layers prepared under various sputtering conditions is provided.

DS 9.30 Mon 15:00 Poster D1

The optical properties of boron carbide near boron K-edge inside periodical multilayers — •Dmitriy Ksenzov, Christoph Schlemper, and Ullrich Pietsch — University of Siegen, Walter-Flex Str. 3, 57068, Siegen, Germany

Multilayer mirrors made for the use in the wavelength range near K-edge of boron (˜188eV) are of great interest for X-ray fluorescence analysis of boron content in doped semiconductors, plasma diagnostics, astronomy and lithography. Moreover, multilayer mirrors composed by a metal and a low Z element like boron are used as optical elements in both the soft x-ray spectral range as well as at higher photon energies on 3rd generation synchrotron beamlines.

Using an energy-resolved photon-in-photon-out method we reconstructed the optical data from energy dependence of both integrated peak intensity and FWHM of the 1st order ML Bragg peak measured at the UHV triple axis soft-x-ray reflectometer at BESSY II. The experiments clearly demonstrate that the peak shape of the ML Bragg peak is most sensitive to any kind of electronic excitation and recombination in solid.

The soft-ray reflectivity can give detailed information for MLs with thickness up to several tens of nanometers. In addition, measurements close to a resonance edge probe the chemical state of the respective constituent accompanied with a high sensitivity of changes close to the sample surface.

DS 9.31 Mon 15:00 Poster D1

Spectroscopic Ellipsometry Investigation of Ultrathin Nb_2O_5 and Nb_2O_5/Al_2O_3 Layers — Marion Friedrich[1], Yue Huang[2], Yan Xu[2], Shi-Jin Ding[2], Li Ding[1], Ovidiu Gordan[1], and •Dietrich R. T. Zahn[1] — [1]Semiconductor Physics, Chemnitz University of Technology, D-09107 Chemnitz, Germany — [2]State Key Laboratory of ASIC and System, Department of Microelectronics, Fudan University, Shanghai 200433, China

Since amorphous Nb_2O_5 films have unique properties, they are widely used as optical interference filters, O_2 sensors and electrochromic material. Also, there is considerable interest in using it as a high permittivity dielectric to replace gate insulators and integrated capacitors. The high k/low k combination of Nb_2O_5/Al_2O_3 is a good candidate to implement the "VARIOT" concept in nonvolatile memory devices. Single Nb_2O_5 layers and Nb_2O_5/Al_2O_3 double layers on silicon were characterised by variable angle spectroscopic ellipsometry in the spectral range from 0.74 eV to 5 eV and by means of vacuum ultraviolet ellipsometry up to 9.8 eV at 67.5° angle of incidence at the synchrotron source BESSY. For the Nb_2O_5 layers the thickness and optical constants were determined. Furthermore, the influence of annealing on the optical properties and the band gap was investigated.
All samples were prepared by atomic layer deposition on HF cleaned silicon substrates at 300°C. The precursors for Nb_2O_5 and Al_2O_3 are $Nb(OEt)_5$ and $Al(CH_3)_3$, together with H_2O, respectively. The base pressure was 2.3×10^2 Pa. Post-deposition annealing was performed in N_2 ambient for 30 seconds at temperatures between 500°C and 800°C.

DS 9.32 Mon 15:00 Poster D1

Vibrational Modes of thin Silicon Membranes — •Reimar Waitz[1], Olivier Schecker[1,2], and Elke Scheer[1] — [1]Universität Konstanz, Germany — [2]jetzt Robert Bosch GmbH

Membranes with thicknesses of a few hundred nanometers and macroscopic lateral size are interesting systems to study the mechanical properties of solids on various length scales. In our experiment a piezo is used to couple in vibrations, which can be observed with a white light interferometer using stroboscopic light. This way we image transverse modes of frequencies up to 12 MHz. The influence of strain on the the dispersion relation is investigated by applying a pressure difference between both sides of the membrane.

DS 9.33 Mon 15:00 Poster D1

Preparation and investigation of epitaxial grown $CaRuO_3$ / $SrTiO_3$/ $CaRuO_3$ - structures — •Janine Fischer, Veit Grosse, Andreas Siebert, Frank Schmidl, and Paul Seidel — Friedrich-Schiller-Universität, Institut für Festkörperphysik, Helmholtzweg 5, 07743 Jena

We deposited layer systems of $CaRuO_3$ / $SrTiO_3$ / $CaRuO_3$ on $LaAlO_3$ using PLD by variation of the $SrTiO_3$ film thickness. The prepared layer systems were characterised via X-rays and AFM. We prepared capacitor structures from these systems after optimisation of the preparation parameters - e.g. substrate temperature, laser energy and oxygen pressure. The temperature dependence of the conductivity and the dielectric properties of the $SrTiO_3$ layers from these structures were investigated. In addition we present first measurements.

DS 9.34 Mon 15:00 Poster D1

Properties of YSZ thin films prepared by RF sputter deposition using a ceramic target — •Benjamin Pachner[1], Angelika Polity[1], Sven Ole Steinmüller[2], and Jürgen Janek[2] — [1]I. Physikalisches Institut, Justus-Liebig-Universität Giessen, Heinrich-Buff-Ring 16, 35392 Giessen, Germany — [2]Physikalisch-Chemisches Institut, Justus-Liebig-Universität Giessen, Heinrich-Buff-Ring 58, 35392 Giessen, Germany

Yttria-stabilized zirconia (YSZ) as an oxygen ion conductor is widely used in technical applications like solid oxide fuel cells for example. The question of film stability and structure is important for increasing the efficiency of these films. In this work YSZ thin films have been prepared by radio frequency (RF) sputter deposition on float glass substrates using a ceramic YSZ target doped with 9.5 mol% yttria and argon as sputtering gas. Several process parameters such as substrate temperature, RF power level, process gas flow rate and the amount of additional oxygen as reactive gas have been varied. The influence of these variations on the structure of the YSZ thin films has been investigated using (among others) scanning electron microscopy (SEM), X-ray diffraction, and optical absorption spectroscopy.

DS 9.35 Mon 15:00 Poster D1

Characterization of magnetron sputtered doped amorphous Silicon films — •Frank Nobis, Philipp Schäfer, Hartmut

Kupfer, Frank Richter, and Dietrich R. T. Zahn — Institute of Physics, Chemnitz Univ. of Technol., 09107 Chemnitz, Germany

Thin film techniques provide excellent capabilities to develop low cost solar cell technologies using amorphous silicon (a-Si). From many research groups a substitutional doping of a-Si films was demonstrated. In contrast to the doping of mono-/polycrystalline Si the doping efficiency is very low, i.e. only a few percent of the chemically incorporated dopants are electrically active. Therefore, an improved doping efficiency is one of the main goals of current investigations.

We have used pulsed d.c. magnetron sputtering to deposit phosphorus- and boron-doped amorphous silicon films. Heavily doped monocrystalline Si targets (n^+, p^+) were sputtered using Ar and Ar/H process gas. The electrical properties and the chemical composition of the films have been characterized by four point probe measurements and secondary ion mass spectrometry (SIMS), respectively. The Raman spectroscopy yielded information about the film structure. The hydrogen incorporation into the Si films was determined by Fourier-transform infrared spectroscopy (FTIR). The film properties will be discussed with respect to the dopant incorporation and to the deposition process parameters.

DS 9.36 Mon 15:00 Poster D1

Mechanical and tribological properties of thin sputtered a-C and CNx layers on polymer substrates — •Zdenek Stryhal[1], Arndt Schumann[2], Hartmut Kupfer[1], Frank Richter[1], and Jens Sumpf[2] — [1]Chemnitz University of Technology, Faculty of Natural Sciences, Reichenhainer Straße 70, D-09126 Chemnitz, Germany — [2]Chemnitz University of Technology, Faculty of Mechanical Engineering, Reichenhainer Str. 70, D-09107 Chemnitz, Germany

Amorphous carbon layers in many forms have been studied for decades and were already used in many industrial applications. These carbon layers are often used due to their good protecting, low friction and low wear properties. PACVD techniques based on discharge in hydrocarbons or hydrogen/hydrocarbon mixture is mostly used and studied. We have studied amorphous carbon and nitrogen doped carbon layers prepared by pulsed DC magnetron sputtering of graphite in argon and argon/nitrogen gas mixture. These layers were deposited on various polymer substrates that are in use in industrial transport systems. Properties like intrinsic stress, adhesion, wear resistance, friction coefficient and surface topography have been investigated. Friction and wear tests were made at conditions similar to those we expect in real transport systems. The aim of the work is to reduce energy consumption by reducing friction losses and by extending durability of coated polymer parts.

DS 9.37 Mon 15:00 Poster D1

Growth and characterization of a copper/cobalt heterostructure on Cu(100) — •Philipp Kloth, Martin Wenderoth, Henning Prüser, and Rainer G. Ulbrich — IV. Physikalisches Institut, Georg-August Universität Göttingen

The copper/cobalt/copper heterostructure is a long known system for the research on quantum well oscillations in thin films [1, 2]. Preparing this system one has to find a trade-off between flat interfaces and intermixing of Co and Cu. We performed a detailed structure analysis for every step of the growth sequence. In the need of sufficient flat interfaces and surfaces one must conduct additional annealing steps after each deposition process. To avoid intermixing the evaporation is done at 80 Kelvin. Low energy electron diffraction (LEED) experiments show an epitaxial deposition. In order to find the appropriate annealing temperature we analyze the surface with auger electron spectroscopy (AES) so that intermixing can be neglected. Scanning tunneling microscopy analysis indicates a successful preparation process: we observe large flat areas. But in comparison to our AES setup (SPECS ErLeed) high resolution STM topographies show that cobalt tends to intermix with the copper film even for rather low heating temperatures. This work is supported by the SFB 602 TP A3.

[1] J. E. Ortega et al., Phys. Rev. Lett. 69, 844 (1992)

[2] T. Uchihashi, Phys. Rev. B 78, 033402 (2008)

DS 9.38 Mon 15:00 Poster D1

Deposition of multi-structural biocompatible thin films with an antimicrobial effect by pulsed magnetron sputtering — •Vitezslav Stranak[1,2], Marion Quaas[1], Martin Cada[2], Zdenek Hubicka[2], Carmen Zietz[3], Kathleen Arndt[4], Rainer Bader[3], Andre Podbielski[4], and Rainer Hippler[1] — [1]University of Greifswald, Institute of Physics, Felix-Hausdorff-Str. 6, 17489 Greifswald, Germany — [2]Academy of Sciences of the Czech Rep., Institute of Physics, Na Slovance 2, 18221 Praha 8, Czech Republic — [3]University of Rostock, Department of Orthopaedics, Doberaner Str. 142, 18057 Rostock, Germany — [4]University of Rostock, Dept. of Med. Microbiol., Vir. and Hyg., Schillingallee 70, 18057 Rostock, Germany

The aim of our work is to produce materials and surfaces for medical devices such as endoprosthetic implants, which combine good cellular adhesion of osteoblasts at the surface with distinguished antimicrobial effects. Our actual approach is to insert Cu as a metal with known antimicrobial properties into the surface of titanium substrates. Crystallographic phases of deposited thin films are investigated by grazing incidence x-ray diffractometry (XRD) and chemical composition is estimated by x-ray photoelectron spectroscopy (XPS). Plasma properties are characterized by time-resolved Langmuir probe measurement, ion particle flux and total energy flux measurements. The combination of these diagnostic methods enables an extensive characterization of the films and also agents responsible for formation of thin films. The work is supplemented by measurements of copper release and antimicrobial effects to give a survey of bio-properties of the thin films.

DS 9.39 Mon 15:00 Poster D1

Structural and electrical properties of sol-gel derived Ge nanocrystals in thin SiO2 layers — •Sebastian Knebel, Agathi Kyriakidou, Hartmut Bracht, Harald Rösner, and Gerhard Wilde — Institut für Materialphysik, WWU Münster, Wilhelm-Klemm-Str. 10, 48149-Münster, Germany

A sol-gel based method for the synthesis of germanium nanocrystals (Ge-nc) in thin amorphous silicon dioxide (SiO2) films on silicon is presented. The synthesis process consists of a wet chemical coating step of Si substrate wafers and annealing steps under both oxidizing and reducing atmosphere. Size, structure and local distribution of the Ge-nc were studied by means of conventional and high-resolution transmission electron microscopy (HRTEM).

The structural properties are dependent on the thickness of the thin film as well as on the temperatures and times used in the annealing steps. Analysis of the thin glass films with energy dispersive x-ray spectroscopy (EDX) shows that Ge migrates to both the Si substrate and the free SiO2 surface. Capacitance-voltage (CV) measurements reveal a hysteresis indicating a trapping of charges in the glass layer.

DS 9.40 Mon 15:00 Poster D1

Focusing Neutron Beams to Sub-Millimeter Size — •roxana valicu and peter böni — Physik-Department E21, Technische Universität München, D-85747 Garching, Germany

Focusing neutron guides are a well-established means to significantly increase the neutron flux for the investigation of small samples or samples subject to extreme conditions such as pressure or high magnetic fields. Parabolic and elliptic guides can focus the beam in a single point beyond the guide exit with well defined beam characteristics and a gain in intensity of over 30 compared to a non-focused beam. Focusing guides find applications in elastic and inelastic neutron scattering as well as in neutron imaging to increase the spatial resolution and for magnification. The aim of the Monte Carlo simulations using McStas was to produce focal spots with a diameter of the order of 0.1 mm using supermirrors with large angles of reflection. We will discuss the results of our simulations, i.e. the gains obtained, their variation with wavelength as well as the evolution of the beam size.

DS 9.41 Mon 15:00 Poster D1

Synthesis and characterization of ion-conducting lithium phosphorus oxynitride thin Films — •Eric Hofmann, Thomas Leichtweiss, Angelika Polity, and Bruno K. Meyer — Justus-Liebig- Universitaet Giessen, I. Physikalisches Institut, Heinrich-Buff-Ring 16, 35392 Giessen, Germany

Transparent amorphous lithium phosphorus oxynitride (LiPON) thin films can be used in smart windows as solid Li+-ion-conductors. Our films were deposited by RF-sputtering from a ceramic Li3PO4 target in pure N2-atmosphere on glass substrates, the film thickness is typically 100 nm. Our aim is to optimize the deposition parameters in view of the ion-conductivity.

The deposition parameters such as the deposition rates, the film stoichiometry and the morphology were studied by X-ray reflection, photo electron spectroscopy and AFM-microscopy. The dependence of the ion-conductivity on the deposition parameters was measured by impedance spectroscopy using InCu|LiPON|InCu sandwich structures.

DS 9.42 Mon 15:00 Poster D1

Characterization of Ion- bombardment induced modifications of periodic La/B_4C-multilayer-mirrors for the reflection of soft X-ray radiation — •Fabian Merschjohann[1], Maike Lass[1], Lennart Gorholt[1], Marc D. Sacher[1], Franz Schäfers[2] und Ulrich Heinzmann[1] — [1]Molecular and Surface Physics, Bielefeld University, D-33615 Bielefeld — [2]Helmholtz-Zentrum Berlin für Materialien und Energie, Elektronenspeicherring BESSY II

The applicability of reflective optical components for the soft X-Ray region depends on the existence of multilayer-optics. Therefore stacks of alternating layers of two materials with different refractive index are applied. For the photon energy range of 100 - 190 eV Lanthanum (La) is favoured as the absorber material and Boroncarbide (B_4C) as the spacer material. Thin periodic layer systems of those materials with double layer periods of 5.6 nm have been produced by UHV Electron Beam Evaporation. The layer thickness is controlled by in-situ X-Ray Reflectometry. The purity and the stoichiometry of the layers has been analyzed by electron beam induced in-situ Auger Spectroscopy. Ion Polishing of each interface should diminish the interface roughness and thus enhance the reflectivity. The modification of the La- and B_4C-layers due to ion bombardment has been investigated by the in-situ Auger Spectroscopy, ex-situ X-Ray Diffraction and at-wavelength reflectivity measurements by use of Synchrotron radiation at the BESSY II facility. Effects of compaction, mixing, sputter-etching and smoothing have been found. The modifications can be influenced by varying the kinetic energy of the ions and/or the duration of the treatment.

DS 9.43 Mon 15:00 Poster D1

X-ray waveguides fabricated by thin film techniques — •Sven Philip Krüger, Giewekemeyer Klaus, Kalbfleisch Sebastian, Henrike Neubauer, and Tim Salditt — Georg-August Universität, Institut für Röntgenphysik, 37075 Göttingen, Deutschland

Waveguides can be used for spatial and coherent filtering of x-rays. We present a two-component waveguide design [1] of enhanced transmission efficiency at carbon guiding layer cross-sections up to sub-10 nm fabricated by magnetron sputtering. The transmission is enhanced by choosing an appropriate molybdenum interlayer. At the same time a strongly absorbing germanium cladding allows for short waveguide lengths which lead to an enhanced efficiency of the waveguide. We used an arrangement of two short waveguide slices to obtain an two-dimensionally confining waveguide with an effective source size of sub-15 nm^2. A first imaging experiment of a test pattern is presented and the images are reconstructed by holographic and iterative phase retrieval algorithms.

[1] T. Salditt et al, Phys. Rev. Lett. 100, 184801, (2008).

DS 9.44 Mon 15:00 Poster D1

Multilayer Bragg Fresnel Zone Plate for coherent HHG radiation — •Christian Späth[1], Michael Hofstetter[2], Jürgen Schmidt[1], Ferenc Krausz[1,2], and Ulf Kleineberg[1,2] — [1]Fakultät für Physik, Ludwig Maximilians Universität München, Garching, Germany — [2]Max Planck Institut für Quantenoptik, Garching, Germany

Coherent Diffractive Imaging in the (soft) X-ray regime is an emerging new lens-less X-ray microscopy technique with the future potential of molecular or even atomic resolution, because it is ultimately limited by the wavelength of the illuminating radiation and not by the imaging quality of the x-ray lens. However, this technique depends on the availability of coherent x-ray sources as well as optics for spectral filtering and focusing. We describe the development fabrication and testing of a reflective multilayer Bragg Fresnel phase zone plate for focusing coherent XUV radiation at 13 nm wavelength from a High Harmonic Generation source. This x-ray optical device serves for spectral filtering as well as sub-micron focusing of the HH spectrum in a single element for largely reduced losses. Large zone plate structures (conventional, spiral) matching the HH beam size are recorded by e-beam lithography in ultrathin HSQ e-beam resist and over-coated with a reflective Mo/Si multilayer by Ion Beam Deposition. By accurately matching the groove depth of the diffractive structure to odd multiples of the quarter Bragg wavelength, the total diffraction efficiency can be improved by a factor of 4 theoretically compared to amplitude structures.

DS 9.45 Mon 15:00 Poster D1

Preparation of a heater and sensor arrangement on Si_3N_4 thin membranes for in-plane thermal conductivity measurements — •David Hartung, Torsten Henning, and Peter J. Klar — I. Physikalisches Institut, Justus-Liebig-Universität Gießen, Germany

The aim of this work is to characterize the lateral heat flow in a thin material layer on a Si_3N_4 membrane. Thin Si_3N_4 membranes (200 nm thickness, 500 μm × 500 μm) on Si-substrates (200 μm thickness, 2.5 mm × 2.5 mm) fabricated by Plano GmbH are used as substrates for the heater and sensor arrangement. A meandering Ag wire along the middle axis of the membrane serves as an electric heater, three Ag-wires of 5 μm thickness at different distances from, but parallel to the heater wire, serve as temperature sensors. The arrangement was defined by electron-beam-lithography on to the membrane. After a development step thin layers of chrome, working as a primer and then silver as the actual wire material were evaporated on to the structured PMMA. A following lift off step completes the nanofabrication of the wire arrangement on the membrane. (spp 1386)

DS 9.46 Mon 15:00 Poster D1

3ω measurements of thermal conductivity in oxide thin films — •Stefanie Wiedigen[1], Manuel Feuchter[2], Christian Jooss[1], and Marc Kamlah[2] — [1]Institute for Materials Physics, University of Göttingen — [2]Institute for Materials Research II, KIT

Several novel approaches for high- efficiency thermoelectric devices are based on thin film geometries like multilayer structures or nanosized devices. Thereby, the 3ω method is one of a few measurement techniques which allows a reliable determination of thin film thermal conductivity. However, the application of the 3ω method on complex geometries and material combinations needs an extension of the standard evaluation techniques. In this contribution, we analyze the conditions for high precision measurements based on the 3ω method in experiment and numerical simulations. For the thin film configurations investigated here, the heat conduction problem is solved by the numerical finite element method. Techniques for modeling the problem and evaluating the results are under development to study the impact of parameters as heater geometry, film thickness and frequency on the voltage signal. The simulation results are compared with the measured frequency spectrum of the ac voltage determined by a 4 terminal geometry. The measurements are performed for Manganite and Cobaltate thin films as promising new thermoelectric materials on $SrTiO_3$ and MgO substrates with different bulk thermal conductivity. Our results are the first steps for an optimization of the measurement configurations and the evaluation of the applicability of common analytical solutions.

DS 9.47 Mon 15:00 Poster D1

Modelling thermoelectric properties of ZnO/ZnS multilayer systems with a network model — •Florian Gather, Gert Homm, Markus Piechotka, Christian Heiliger, Peter J. Klar, and Bruno K. Meyer — I. Physikalisches Institut, Justus-Liebig-University, Heinrich-Buff-Ring 16, 35392 Giessen

Two different types of ZnO/ZnS multilayer systems are investigated. The first is a multilayer system with alternating layers of ZnO and ZnS. The second one consists of a chequer-board pattern of the two materials. For the modeling of the electric and thermal properties of both systems a two-dimensional network model was used. The spatial properties such as layer thicknesses and interface roughness are translated into a pixel grid. In order to calculate the thermal or electric resistance, each pixel cell consists of a node with a local resistance connected to the four nearest-neighbour pixel cells. The calculated total resistance of the network is then converted into an either electric or thermal conductance of the multilayer structure. To calculate the effective Seebeck-coefficient of the system a temperature difference between the contacts is applied. Then the individual temperature differences between the nodes are determined and used to calculate the local Seebeck-voltages. These are now implemented into the electric resistance network via voltage sources. To determine the effective Seebeck-coefficient of the multilayer structure the voltage between the contacts of the multilayer structure is calculated and divided by the applied temperature difference. The influence of the spatial parameters on the thermoelectric properties is studied. (SPP 1386)

DS 9.48 Mon 15:00 Poster D1

Ab initio investigations of ZnO/ZnS interfaces — •Michael Bachmann, Robert Henrich, and Christian Heiliger — I. Physikalisches Institut, Justus Liebig University Giessen, D-35392, Germany

ZnO/ZnS nanostructures are a promising material for thermoelectric applications due to the expectation of a strong phonon scattering at the interface but a high transmission of electrons through the interface. Therefore, the atomic positions, the coupling of the atoms, and the electronic states at the interface are of special interest. We present ab initio calculations of ZnO/ZnS interfaces in wurzite structure for different boundary conditions based on a pseudopotential method. We calculate the equilibrium positions of the atoms at the interface and the coupling between them.(SPP 1386)

DS 9.49 Mon 15:00 Poster D1

Thermoelectric properties of silicon nano pillars — •Andrej Stranz, Ünsal Sökmen, Andreas Waag, and Erwin Peiner — Institute of Semiconductor Technology, Braunschweig, Germany

In order to establish silicon as a efficient thermoelectric material, its high thermal conductivity has to be reduced which is feasible, e.g., by nano structuring. Therefore, in this study Si-based sub-micron pillars of various dimensions were investigated. Using anisotropic etching followed by thermal oxidation we could fabricate pillars of diameters < 500 nm, about 25 *m in height with aspect ratios of more than 50. The distance between the pillars was varied from 500 nm to 10 micron. Besides the fabrication and structural characterization of sub-micron silicon pillars, and adequate metrology for measuring their thermoelectric properties was implemented. Commercial tungsten probes and self-made gold probes, as well as Wollaston wire probes were used for electrical and thermal conductivity, as well as Seebeck voltage measurements on single pillars in a scanning electron microscope equipped with nano manipulators.

DS 9.50 Mon 15:00 Poster D1

Thermoelectric properties of hot wall deposited thin SnS films — •Dzianis M. Unuchak[1], Vasil A. Ivanov[2], Valeriy F. Gremenok[2], and Klaus Bente[1] — [1]Institut für Mineralogie, Kristallographie und Materialwissenschaft, Universität Leipzig, Scharnhorststr. 20, 04275 Leipzig, Germany — [2]State Scientific and Production Association "Scientific-Practical Materials Research Centre of the National Academy of Sciences of Belarus", P. Brovka str., 19, 220072 Minsk, Belarus

Polycrystalline ingots of SnS was directly synthesized from a stoichiometric mixture of 99.999 % purity Sn and S in a vacuum-sealed quartz ampoule. Thin SnS films were deposited by hot wall technique on glass and molybdenum substrates under an ambient pressure of $5*10^{-6}$ mbar. The elemental composition of the obtained films was determined to be stoichiometric (SEM-EDX). The crystal structure and crystalline phases of the samples were studied by X-ray diffraction (Siemens D-5000 diffractometer with CuK_α radiation). The obtained films were polycrystalline, monophase in nature and had orthorhombic crystal structure. The films on glass were highly oriented along (001) plane whereas films on molybdenum showed SnS phase with different orientation. The as-prepared films show *p*-type electrical conductivity confirmed by the thermoelectric probe measurement. The value of Seebeck coefficient was about 1000 and 400 μV/K for films on glass and Mo, respectively.

DS 9.51 Mon 15:00 Poster D1

Properties of thin films and bulk of $\mathbf{Pb_{1-x}Sn_{1+x}X_2}$ (X=S, Se) mixed crystals — •Vera Lazenka[1], Klaus Bente[1], and Valery Gremenok[2] — [1]Institut für Mineralogie, Kristallographie und Materialwissenschaft, Universität Leipzig, Scharnhorststr. 20, 04275 Leipzig, Germany — [2]State Scientific and Production Association "Scientific-Practical Materials Research Centre of the National Academy of Sciences of Belarus", P. Brovka str., 19, 220072 Minsk, Belarus

Mixed crystals of the galena-herzenbergite-system implying intermediate $\mathrm{PbSnS_2}$ are perspective for thermoelectric, photovoltaic etc. materials. In addition to the Pb-Sn-substitution the replacement of S by Se and Te is studied, taking in account that thermoelectrical properties of e.g. PbX are improved by the substitution of S for Se and Te. The work aims to investigate the effect of anionic and metal atom substitutions in SnX - $\mathrm{PbSnX_2}$ on structure and optical and electrical properties. For target synthesis Sn, Pb, S and Se (99.998 %) were reacted in vacuum-sealed quartz ampoules. Because of the thermoelectrical properties improvement caused by metal impurities in galena, also natural PbS is used. Thin films were prepared from powder material by hot wall evaporation method at $7*10^{-6}$ mbar on glass substrates at 200-350 °C. $\mathrm{Pb_{1-x}Sn_{1+x}X_2}$ (X=S, Se) characterized by XRD and EPMA and effects of Pb-Sn and S-Se ratios on the thermopower are presented.

DS 9.52 Mon 15:00 Poster D1

Thermoelectric properties of ball-milled and subsequent short-term sintered $\mathbf{In_xCo_4Sb_{12}}$ skutterudites — •Andreas Sesselmann, Ralf Hassdorf, Lothar Böttcher, Christian Stiewe, Andreas Schmitz, and Eckard Müller — German Aerospace Center (DLR), Institute of Materials Research, 51170 Cologne, Germany

For more than a decade, $\mathrm{CoSb_3}$ has been widely studied as a promising thermoelectric (TE) material at intermediate temperatures. High thermoelectric figure of merit (ZT) in this material system can be achieved by filling guest atoms known as rattlers. One of the best improvements in ZT is reported when In is used as a filler atom leading to a $\mathrm{ZT_{max}}$ of about 1.2 at 575 K [1]. Another approach to lower the lattice thermal conductivity is by nano-structuring which leads to increased phonon scattering at the grain boundaries. The approach in this study is based on planetary ball milling, which allows for grain sizes on the nanometer scale and subsequent compaction by short-term sintering in favour of grain growth confinement. Phase homogeneity of the bulk material has been probed by XRD and EDX. TE properties (i.e. electrical conductivity, Seebeck coefficient, thermal conductivity) have been analyzed in the temperature range from 300 K to 700 K. The functional homogeneity of the samples was checked by Potential-Seebeck Microprobe (PSM). Based on these results, the combined effect of In filling and nano-structuring on the TE properties will be discussed.

[1] T. He *et al.*, Chemistry of Materials, 2006, 18, 759-762

DS 9.53 Mon 15:00 Poster D1

Complex Chalcogenides for Thermoelectrics: Microstructural-Property Relationship — •Susanne Perlt and Thomas Höche — Leibniz Institute of Surface Modification, Permoserstrasse 15, D-04318 Leipzig, Germany

The quaternary compound $\mathrm{AgPb_{18}SbTe_{20}}$ (LAST) is a typical high-temperature thermoelectric material. The manufactoring process needs to be controlled in such a way, that the figure of merit, ZT [1], gets maximized. In this respect, a high electronic conductivity σ, a high thermopower S, and a low thermal conductivity κ are crucial. The high thermoelectric performance of LAST is assumed to be caused by the nanoscale precipitates formed by spinodal decomposition [2]. Based on properties monitored by a Seebeck probe, structure-property relationships are studied by SEM and TEM analysis. Site-specific lift-out of TEM lamellae from thermoelectrically characterised samples is made by focused ion beam (FIB) machining. Composition analyses, phase analyses (via electron diffraction) and element distributions are done by energy-dispersive X-ray spectrometry.

[1] D. Bilc et al., Phys. Rev. Lett. **93**, 146403 (2004)
[2] M.-K. Han et al., Chem. Mater. **20**, 3512 (2008)

DS 10: Plasmonics and Nanophotonics I (Joint Session DS/O/HL)

Time: Tuesday 10:30–13:00 Location: H2

DS 10.1 Tue 10:30 H2

Electrochemically tunable photonic metamaterial — •Lihua Shao, Stefan Linden, Matthias Ruther, Jörg Weissmüller, and Martin Wegener — Institut für Nanotechnologie and DFG-Center for Functional Nanostructures (CFN), Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany

We report experiments to combine two approaches for designing functional nanomaterials. Photonic metamaterials provide a strategy for obtaining unconventional optical response - in the extreme, negative refractive indices - by lithographically structured elements like arrays of split-ring resonators (SRR). Nanomaterials with tunable electronic structure exploit large specific surface area of metal nanostructures to tune the surface properties through the controlled space-charge regions for tuning macroscopic properties. The combination is a photonic metamaterial in which the space-charge at the surface of SRR is controlled via an applied potential, leading to a tunable optical resonance. We report first results support this concept. SRR structures with resonance frequencies in the near infrared are immersed into aqueous electrolytes as working electrode in an electrochemical experiment.

Varying the electrode potential, E, induces a space-charge layer at the metal surface as part of the electrochemical double-layer. We find the resonance frequencies vary linearly, reversibly, and reproducibly with E, with a blue shift for negative potential. A tentative explanation is based on the effective thickening of the SRR by the excess electrons, which changes the SRR aspect ratio. The observation of larger frequency shift for thinner SRR's is compatible with this scenario.

DS 10.2 Tue 10:45 H2

Mixing colours like nature — •Mathias Kolle, Maik Scherer, Pedro Cunha, Fumin Huang, Jeremy Baumberg, and Ullrich Steiner — Cavendish Laboratories, University of Cambridge, UK

Biomimetic attempts to produce novel photonic structures have attracted increasing research interest in recent years. Nature offers us an enormous amount of multifunctional micro- and nanostructures, that provide outstanding, distinctive, dynamic and tailored colouration. A "brilliant" example is the indonesian butterfly *papilio blumei*, whose wing scales are covered with 5-10μm wide concavities, that are cladded with a perforated cuticle multilayer. The regularly shaped multilayer structure gives rise to very impressive colour mixing effects, accompanied by controlled change in light polarisation.

We have successfully replicated the intricate photonic structure of *papilio blumei* on the cm^2-scale in four simple steps involving colloidal templating, electrochemical growth and atomic layer deposition. A small conceptual modification of the original photonic structure leads to a completely different optical effect. Any freely chosen colour and its complementary hue can be separated and reflected into different directions while conserving a particular polarisation effect.

Since the procedures are easily up-scaleable, these biomimetic photonic structures have a huge potential for industrial applications in security printing, encoding of information, non-emissive display technology and other fields where distinct colours play an important role.

DS 10.3 Tue 11:00 H2

Optical properties of carpets of randomly grown silicon nanowires on glass — •Gerald Brönstrup and Silke Christiansen — Institut für Photonische Technologien e.V., Abt. Halbleiter-Nanostrukturen, 07745 Jena

Silicon Nanowires [SiNWs] have attracted much attention in the recent years as possible future building blocks for field effect transistors, sensors, photo detectors and solar cells. For the latter SiNWs grown on a cheap substrate like glass is of special interest. To build solar cells with high efficiencies a high absorption is mandatory. We present a study of the influence of the diameter on the reflection, transmission and absorption spectra of carpet like assembly of SiNWs grown on glass.

We grew SiNWs on glass using gold colloids of different fixed diameters to achieve a control over the diameter of the SiNWs. Then we measured the reflection R and transmission T using an integrating sphere. The absorption A was calculated using the simple formula A=1-T-R.

For a better understanding of the underlying physics of the absorption happening in SiNWs with diameters much smaller than the wavelength of the visible light we present a statistical model based on scattering cross sections calculated for single SiNWs using Mie-theory.

DS 10.4 Tue 11:15 H2

Suppressed transmission through ultrathin metal films by subwavelength hole arrays — •Julia Braun[1], Bruno Gompf[1], Uwe Huebner[2], and Martin Dressel[1] — [1]1. Physikalisches Institut, Universität Stuttgart, Pfaffenwaldring 57, 70550 Stuttgart — [2]IPHT Jena, Albert-Einstein-Straße 9, 07745 Jena

If an opaque metal film is periodically perforated by tiny subwavelength holes, extraordinary high transmission is observed [1]. We investigate the transmission through subwavelength hole arrays (SWHA) in ultrathin semitransparent Au films with various periodicities and hole diameters and observe the opposite behavior: less light is transmitted through the pierced metal compared to the closed film. The samples were fabricated by optical interference and electron beam lithography in 12 nm and 20 nm thick Au films with periodicities between 250 nm and 400 nm, and than characterized in the frequency range 4400 cm^{-1} to 37000 cm^{-1} (0.6 eV to 4.6 eV). The optical properties of SWHA cannot be explained by a pure dielectric function, but show a strong $\vec{k}$-dependent behavior. In ultrathin Au films it is marked by the excitation of strongly damped antisymmetric short range surface plasmons. The obtained dispersion curves perfectly agree with this explanation when the altered dielectric function of the ultrathin Au films is taken into account [2].

[1] T.W. Ebessen, H.J. Lezec, H.F. Ghaemi, T. Thio, and P.A. Wolff, *Nature* **391**, 667 (1998).

[2] J. Braun, B. Gompf, G. Kobiela, M. Dressel, *Physical Review Letters* **103**, 203901 (2009)

DS 10.5 Tue 11:30 H2

Manipulation of fluorescence resonance energy transfer in single plasmonic nanoresonators — •Valerie Faessler, Calin Hrelescu, Sergiy Mayilo, Frank Jäckel, and Jochen Feldmann — Photonics and Optoelectronics Group, Department of Physics and Center for Nano Science (CeNS), Ludwig-Maximilians-Universität München, Amalienstrasse 54, 80799 München, Germany;

We show that fluorescence resonance energy transfer (FRET) between two organic chromophores can be manipulated in plasmonic nanoresonators consisting of two spherical gold nanoparticles.The nanoresonators can be tuned by varying the inter-particle distance or the nanoparticle size. This allows us to selectively modify the decay channels of the chromophores. FRET can be supressed if the molecules are placed in the nanoresonator at a certain distance from the nanoparticle surface. Furthemore we observe spectral shaping and intensity modulation of the fluorophore emision in the nanoresonators [1]. Correlated whitelight Rayleigh scattering and fluorescence microscopy data of the hybrid system are discussed in the framework of generalized Mie theory.

[1] M. Ringler, A. Schwemer, M. Wunderlich, A. Nichtl, K. Kürzinger, T. A. Klar, J. Feldmann Phys. Rev. Lett., 100, 203002 (2008)

DS 10.6 Tue 11:45 H2

Optical antenna thermal emitters — •Jon Schuller[1], Thomas Taubner[1,2], and Mark Brongersma[1] — [1]Stanford University, Stanford, CA, USA — [2]1. Physikalisches Institut, RWTH Aachen, Germany

Optical antennas are a critical component in nanophotonics research[1] and have been used to enhance nonlinear and Raman cross-sections and to make nanoscale optical probes [2]. In addition to their receiving properties, optical antennas can operate in broadcasting mode, and have been used to modify the emission rate[3] and direction [4] of individual molecules.

In these applications the antenna must operate at frequencies given by existing light emitters. Using thermal excitation of optical antennas, we bypass this limitation and realize emitters at infrared frequencies where sources are less readily available [5].

Specifically, we show that the thermal emission from a single SiC whisker antenna is attributable to well-defined, size- tunable Mie resonances. Furthermore, we derive a fundamental limit on the antenna emittance and argue theoretically that these structures are nearly ideal black-body antennas.

1. Schuck, P. J. et al., PRL 94, 017402 (2005).
2. Farahani, J. N., et al., PRL 95, 017402 (2005).
3. Kuhn, S., et al., PRL 97, 017402 (2006).
4. Taminiau, T. H., et al, Nature Photon. 2, 234-237 (2008).
5. Schuller, J.A. et al., Nature Photon. 3, 658-661 (2009).

DS 10.7 Tue 12:00 H2

Spatial Resolved Near Field Interference on Nanooptical Bowtie Antennas — •Pascal Melchior, Daniela Bayer, Christian Schneider, Martin Rohmer, Alexander Fischer, and Martin Aeschlimann — Fachbereich Physik and Research Center OPTIMAS, Technische Universität Kaiserslautern, Erwin-Schrödinger-Str. 46, 67663 Kaiserslautern, Germany

The response of metallic nanostructures is responsible for interference effects of the electric near field in the vicinity of the structure surface. While the incoming electric field vectors are independent in the far field, spectral interference in the near field can occur since the resulting field vectors are not necessarily perpendicular. On the nanostructure configuration of a Bowtie antenna, we show how the superposition of different plasmonic excitation modes leads to a local enhancement of the effective near field depending on the phase relation between the incoming electric field vectors. Via an interferometric superposition of two laser pulses with cross polarized electric fields the near field interference can be directly observed by means of a photoemission electron microscope (PEEM). Spatial switching of the photoemission yield depending on the relative phase between the two superposed laser pulses will be demonstrated.

DS 10.8 Tue 12:15 H2

Interaction effects of gold nanoantenna arrays in the infrared — •Daniel Weber[1], Frank Neubrech[1], Dominik Enders[2], Tadaaki Nagao[2], and Annemarie Pucci[1] — [1]Kirchhoff Institute for Physics, University of Heidelberg, Germany — [2]National Institute for Materials Science, Tsukuba, Japan

Gold nanoantennas are of great interest for applied spectroscopy due to their tuneable plasmonic properties including local electromagnetic (EM) field enhancement (FE). Excited resonantly by EM radiation, they are able to strongly enhance the local EM field. In the past, we exploited this strong effect for surface-enhanced infrared spectroscopy (SEIRS) with gold nanoantennas. We want to further improve the sensitivity of SEIRS by making use of nanoantenna coupling. Coupling may increase local FE but also strongly modify the spectral distribution of the FE, which provides further options for optimum resonance tuning as necessary for specific sensor applications.

We report on the IR optical properties of gold-nanoantenna arrays with different gap sizes and show the relation between plasmonic resonances and geometrical arrangement on the substrate. Stripe-like, polycrystalline gold nanoantennas (nanorods) with rectangular cross-sections were produced by electron beam lithography on silicon wafers. IR measurements were performed by micro-spectroscopy in our laboratories and at the synchrotron light source ANKA (Karlsruhe Institute of Technology). Special focus is on the preparation of very small gaps between the tip ends of nanorods, where the highest local FE is expected.

DS 10.9 Tue 12:30 H2

Structural and Optical Properties of Gold and Iron Nanowires — •Piotr Patoka[1,2], Georgios Ctistis[3], Michael Hilgendorff[1], and Michael Giersig[1] — [1]Freie Universität Berlin — [2]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH — [3]University of Twente, MESA+ Institute & Dept. of Science and Technology, Complex Photonic Systems (COPS), Enschede, The Netherlands

Plasmonic nanostructures gained a tremendous interest during the last decade due to their structural and optical properties, which make them promising materials for opto-electronic as well as bio-sensing-applications.

Here we will present results on gold and iron nanowires prepared by means of nanosphere lithography as a cheap method of preparation of large areas of such nanostructures. The 30nm thick lines with 440nm in periodicity have been characterized with atomic force microscopy and scanning electron microscopy. The investigation showed strong influences of the preparation steps to the final structure. For optical investigation UV-VIS-NIR spectrometry and scanning near field optical microscopy have been used showing extraordinary light transmission.

DS 10.10 Tue 12:45 H2

Surface Plasmon Resonance Coupling on Magnetically Capped Gold Nanorods — •Gillian Doyle and Dominic Zerulla — Plasmonic and Ultrafast Optics Group, School of Physics, University College Dublin, Belfield, Dublin 4, Ireland

Nanorods compared to their spherical counterparts exhibit enhanced sensitivity and are used for a wide variety of applications from biosensing to solar cells. The presence of two resonance peaks in their scattering spectra allows their two geometrical axes, the longitudinal and transverse axes to be separately distinguished. In this research we use iron capped gold nanorods with geometrical dimensions in the range of 60 x 700 nm. Coupling of the surface plasmons between the two axes is investigated both in multiple particle and single particle experiments and the effect of the proximity of particles to each other and their associated coupling is considered. In the single particle experiments a 532 nm laser beam is used to optically trap and manipulate a nanorod, while coupling white light to the setup allows Mie Scattering Spectroscopy (MSS) to be performed on a single particle. Large sample MSS experiments provide more intense signals for detection and give an insight into phenomena occurring at the surface of the nanoparticle [1]. In addition, the intensity of the scattering cross section by these nanorods is examined by magnetically manipulating the particles themselves and opening a novel method of optimum signal detection of SP resonances on nanorods.

[1] G Doyle, D. Zerulla, Applied Physics A, Vol 89, No. 2, 2007

DS 11: [O] Plasmonics and Nanophotonics II (Joint Session DS/O/HL)

Time: Tuesday 15:00–16:30 Location: H2

DS 11.1 Tue 15:00 H2

Nanolocalization of time-reversed optical fields propagating in random scattering media — •Dominik Differt[1], F. Javier Garćia de Abajo[2], and Walter Pfeiffer[1] — [1]Fakultät für Physik, Universität Bielefeld, Universitätstr. 25, 33516 Bielefeld, Germany — [2]Instituto de Optica, CSIC, Serrano 121, 28006 Madrid, Spain

The far field emission pattern of a nanoscale light emitter positioned in a nanoscale random scattering environment contains information about the localized emission. Because of the reciprocity of electromagnetic wave propagation time-reversing the outgoing wave creates an excitation that propagates back to the emitter and localizes on a sub-diffraction length scale. The electromagnetic response of a random scattering environment is calculated based on a multiple scattering approach. The here investigated scattering environment is characterized by a geometrical hierarchy. On a subwavelength scale the emitter is surrounded by metal nanoparticles acting as a random antenna coupling radiation to the far field. On the scale of tens of microns, several wavelengths distance to the emitter, this structure is embedded in randomly distributed dielectric scatterers acting a permeable reverberation shell. The degree of nanolocalization of a time-reversed planar wave component of the outgoing scattered wave depends on this geometrical hierarchy and the density of scatterers, i.e. the wave mixing occurring in the reverberation shell.

DS 11.2 Tue 15:15 H2

Towards Nanostructure-Enhanced High-Harmonic Generation — Murat Sivis[1], Katrin Siefermann[2], Yaxing Liu[2], Bernd Abel[2,3], and •Claus Ropers[1] — [1]University of Göttingen, Courant Research Center Nano-Spectroscopy and X-Ray Imaging, Friedrich-Hund-Platz 1, D-37077 Göttingen, Germany — [2]University of Göttingen, Department of Physical Chemistry, Tammannstr. 6, D-37077 Göttingen, Germany — [3]University of Leipzig, Wilhelm-Ostwald-Institute for Physical and Theoretical Chemistry, Linnestr. 2, D-04103 Leipzig, Germany

Recent efforts to utilize optical field enhancements in metallic nanostructures for high-harmonic generation (HHG) have generated significant interest [S. Kim *et al.*, Nature **453**, 575 (2008)]. Using local plasmon resonances, the threshold for HHG can be substantially reduced, allowing for HHG by using unamplified few femtosecond laser oscillators. To date, rather limited information on the characteristics and scaling behavior of the relevant processes is available.

Here, we present the first results of our study on harmonic generation with metallic nanostructures in the presence of a noble gas jet. We demonstrate the significant enhancement of harmonic generation of low orders. Experimental limitations and prospects of the approach are discussed.

DS 11.3 Tue 15:30 H2

Third-Harmonic Generation Spectroscopy in Hybrid Plasmonic Systems — •Tobias Utikal[1,2], Thomas Zentgraf[3], Markus Lippitz[1,2], and Harald Giessen[1] — [1]4. Physikalisches Institut, Universität Stuttgart — [2]Max-Planck-Institut für Festkörperforschung, Stuttgart — [3]NFS Nano-Scale Science and Engineering Center, University of California, Berkeley, USA

In this work we perform third-harmonic generation (THG) spectroscopy in metallic photonic crystals consisting of gold nanowires buried in a dielectric slab waveguide. In these structures particle plasmon polaritons, which are optically excited in the wires, can be hybridized with photonic waveguide modes, which are excited due to the periodic arrangement of the wires. By tailoring the structure geometry the spectrally broad particle plasmon resonance can exhibit an ultra-narrow and pronounced extinction dip. We excite this hybrid plasmonic system with 150 fs laser pulses which can be spectrally tuned over the modulated plasmonic resonance and measure the generated third-harmonic light. The experiments show that it is insufficient to deduce the shape of the THG spectrum from the linear extinction. It is rather essential to consider the full information of the linear response, i.e. amplitude and phase. We find indications that the increased group index and the associated slow light around the extinction dip leads to an increase in the THG signal.

DS 11.4 Tue 15:45 H2

Ultrafast optical nonlinearities in hybrid metal-semiconductor nanostructures — •Parinda Vasa[1], Robert Pomraenke[1], Wei Wang[1], Stephan Schwieger[2], Erich Runge[2], and Christoph Lienau[1] — [1]Carl von Ossietzky Universitaet, Institut fuer Physik, 26111 Oldenburg, Germany — [2]Technische Universitaet Ilmenau, Institut fuer Physik, 98684 Ilmenau, Germany

Understanding and manipulating the interactions between quantum emitters and Surface Plasmon Polaritons (SPPs) is the key to designing and implementing novel nano-optical devices such as nanolasers or ultrafast optical switches. We report the first measurement of an ultrafast optical nonlinearity resulting from the strong interaction between SPPs excited on a gold grating and excitons in either a semiconductor QW or a J-aggregated cyanine dye. The hybrid nanostructures are characterized using far-field linear reflectivity as well as photoluminescence measurements and exhibit enhanced SPP-exciton coupling in the linear optical regime. The experimental results are explained within a phenomenological, coupled oscillator model. The nonlinearity is investigated by low-temperature, angle-resolved, ultrafast pump-probe spectroscopy with 20-fs-time resolution. Due to the strong coupling a significant shift in the resonance wavelength and changes in the response time of the third order nonlinearity of the exciton are observed. Such a strong ultrafast nonlinear interaction between metal and excitons will be of key importance to amplify SPP excitations in such hybrid structures.

DS 11.5 Tue 16:00 H2

Plasmon Hybridization Enhances the Nonlinear Response of Single Metal Nanoparticles — •Thorsten Schumacher[1,2], Kai Kratzer[1,2], David Molnar[1,2], and Markus Lippitz[1,2] — [1]Max-Planck-Institut für Festkörperforschung, Stuttgart — [2]4. Physikalisches Institut, Universität Stuttgart

The optical investigation of single metal nanoparticles is limited to rather large sizes due to their weak influence on focused laser radiation. Therefore it is very difficult to detect small dielectric variations, which is crucial for modern plasmonic nanosensors. We induce small, periodic variations of a nanoparticle's plasmonic properties by a heating pump puls that triggers acoustical breathing oscillations. The particle's response is monitored by a probe pulse. An optical nanoantenna increases the influence of these single dielectric objects on the laser focus. Such an antenna can be implemented by placing a bigger nanoparticle close to the smaller one that is probed.

We will show measurements of single metal nanoparticles' acoustic breathing modes as well as their first antenna enhanced detection. A model of the antenna-effect of plasmon hybridisation is presented. At the end, it allows us to analyze the individual nanomechanical properties of tiny single metal nanoparticles and study plasmonic coupling effects, without averaging over big ensembles.

DS 11.6 Tue 16:15 H2

Enhanced Raman scattering at nanoparticles and gratings with nanoparticles — •Manuel Gonçalves and Othmar Marti — Universität Ulm - Inst. für Experimentelle Physik, Albert-Einstein-Allee 11, 89081 Ulm, Deutschland

Silver and gold nanoparticles of triangular shape in periodic arrays are appropriate templates for molecular detection by means of surface enhanced Raman scattering (SERS). The near-field enhancements may reach 100 and the corresponding Raman electromagnetic enhancements are of the order of 10^8. On the other hand, surface plasmon modes supported in gratings contribute as well to near-field enhancements, and allow an easy excitation of the long-range surface plasmons in the grating.

We show how plasmonic systems built of gratings and nanoparticles can be of interest for SERS, and how strong near-fields may be achieved. SERS measurements done with a confocal Raman microscope permit to study the dependence of near-field intensity on the shape of the particle and on the excitation conditions.

DS 12: Invited Schlecht

Time: Tuesday 9:30–10:15 Location: H8

Invited Talk DS 12.1 Tue 9:30 H8

Preparation methods and thermoelectric properties of PbTe based nanocomposites containing an inclusion phase — Denis Petri[1], Christoph Erk[2], •Sabine Schlecht[2], Ralf Hassdorf[3], Eckhard Müller[3], Gert Homm[4], Markus Piechotka[4], Florian Gather[4], and Peter J. Klar[4] — [1]Freie Universität Berlin, Institut für Chemie und Biochemie, Fabeckstrasse 34-36, 14195 Berlin — [2]Justus-Liebig-Universität Gießen, Institut für Anorganische und Analytische Chemie, Heinrich-Buff-Ring 58, 35392 Gießen — [3]DLR Köln, Linder Höhe, 51147 Köln — [4]Justus-Liebig-Universität Gießen, I.Physikalisches Institut, Heinrich-Buff-Ring 16, 35392 Gießen

With the growing interest of the automotive industies in medium temperature TEGs, lead telluride PbTe and its nanoscale structuring gets in the focus of further material developments. A comparative study on the preparation and the properties of PbTe based nanocomposites will be presented in this contribution. Ball-milling methods were applied for the preparation of different formally ternary and quaternary phases. The thermopower values and the electrical conductivities were evaluated for cold-pressed samples. The changes in the morphologies of the different composites after an annealing step were investigated by SEM and TEM methods. Diffusion processes at the interface of the inclusion and the PbTe matrix seem to play an important role.

DS 13: Thermoelectric Thin Films and Nanostructures I

Time: Tuesday 10:30–13:00 Location: H8

DS 13.1 Tue 10:30 H8

Thermoelectric investigations on nanocomposite PbTe with different inclusions — •Gert Homm[1], Denis Petri[3], Sabine Schlecht[2], and Peter J. Klar[1] — [1]I. Physikalisches Institut, Justus-Liebig-Universität, Gießen, Germany — [2]Institut für Anorganische und Analytische Chemie, Justus-Liebig-Universität, Gießen, Germany — [3]Institut für Chemie und Biochemie, Freie Universität Berlin, Berlin, Germany

We investigated different series of nanogranular so called LAST (LeadAntimonySilverTelluride) samples where either the composition of the inclusion of particles was varied or the PbTe matrix itself was doped isovalently by different elements. Inclusion particles of $BiSbTe_3$, $AgSbBiTe_2$ and $AgSbTe_2$, respectively, were distributed into a nanoparticulate matrix of PbTe by co-ball-milling of the two components and compacting/annealing of the resulting composite material. This is a very easy and economic way of nanostructuring. The resulting nanogranularity of the material is supposed to exhibit a lower thermal conductivity than the corresponding bulk material but possess comparable electrical conductivity. The thermopower and the electrical conductivity was measured in the range of 50-300 K before and after annealing of the specimens. The changes of the thermoelectric properties due to doping of the PbTe matrix as well as of the nanograins will be discussed. The effects of the annealing with respect to structural changes as well as dopant diffusion will be explained. (SPP 1386)

DS 13.2 Tue 10:45 H8

Experimental and theoretical investigations of PbTe-based nanocomposites with different inclusion phases — Denis Petri[1], Christoph Erk[2], Gert Homm[3], Markus Piechotka[3], Peter J. Klar[3], Sabine Schlecht[2], and •Beate Paulus[4] — [1]Freie

Universität Berlin, Institut für Chemie und Biochemie, Fabeckstraße 34-36, 14195 Berlin — [2]Justus-Liebig-Universität Gießen, Institut für Anorganische und Analytische Chemie, Heinrich-Buff-Ring 58, 35392 Gießen — [3]Justus-Liebig-Universitä t Gießen, I. Physikalisches Institut, Heinrich-Buff-Ring 16, 35392 Gießen — [4]Physikalische und Theoretische Chemie, Freie Universität Berlin, Takustraße 3, 14195 Berlin

Nanocomposite thermoelectric materials made by co-ball-milling of lead telluride and an added inclusion phase of Sb_2Te_3, $BiSbTe_3$, Bi_2Te_3 or $AgSbTe_2$ were investigated. A cold-pressing/annealing approach was applied to the resulting powders and the thermopower and the electrical conductivity of the products were measured in the temperature range of 50-300 K. The two quaternary phases $Pb_{10}BiSbTe_{13}$ (n-type) and $Pb_{10}AgSbTe_{12}$ (p-type) show the most promising power factors within the series of nanocomposites investigated. These experimental investigations are supported by first principle calculations for the bulk and the surfaces on the different materials.

DS 13.3 Tue 11:00 H8

Conductivity anisotropy of layered BiTe-SbTe-heterostructures — •Bogdan Yavorsky[1], Nicki Hinsche[1], Martin Gradhand[1,2], Peter Zahn[1], and Ingrid Mertig[1,2] — [1]Martin-Luther-Universität Halle-Wittenberg, Institut für Physik, D-06099 Halle — [2]MPI für Mikrostrukturphysik, Weinberg 2, D-06120 Halle

Transport properties of ordered bismuth and antimony tellurides are studied theoretically based on first-principle electronic structure calculations using a screened Korringa-Kohn-Rostoker Greens function method. The anisotropy of the electron mobility both in the bulk materials and in layered BiTe-SbTe-heterostructures is analyzed within the relaxation time approximation of the Boltzmann theory. The influence of doping on the electrical conductivity is discussed applying the rigid band approximation.

DS 13.4 Tue 11:15 H8

Evidence of Multiphase Nature of β-Zn_4Sb_3 by means of Surface Scanning Techniques — •Titas Dasgupta[1], Christian Stiewe[1], Ralf Hassdorf[1], Lothar Böttcher[1], Hao Yin[2], Bo Iversen[2], and Eckhard Müller[1] — [1]German Aerospace Center (DLR), Institute of Materials Research, Linder Höhe, 51147, Cologne, Germany — [2]University of Aarhus, Department of Chemistry, Langelandsgade 140, DK-8000, Aarhus, Denmark

β-Zn_4Sb_3 has been considered as a promising candidate for thermogenerator applications for long due to its high thermoelectric figure of merit (ZT) reaching up to $\sim$1.3 at intermediate temperatures. The high ZT is a result of the unusually low thermal conductivity (κ) observed in this material. The cause of this low κ is still under debate. Reports on structural analyses reveal a disordered structure with presence of interstitial Zn atoms to be the likely cause of the low κ. Also, soft phonon modes have been observed in this material due to the presence of Sb dimers which can also lead to the observed low κ. Thus the present work investigates the surface homogeneity and microstructure of β-Zn_4Sb_3 based on Seebeck Microprobe (PSM) and Scanning Electron Microscopy (SEM) studies. PSM measurements indicate the presence of local structures with slightly varying but distinct Seebeck (S) values. SEM studies also reveal the presence of local structures arising due to dopant contrast.Based on these observations, the possibility of the presence of multiple phases within β-Zn_4Sb_3 is discussed.

DS 13.5 Tue 11:30 H8

Thermoelectric $CoSb_3$ thin films on amorphous SiO_2 substrates — •Marcus Daniel, Christoph Brombacher, Gunter Beddis, and Manfred Albrecht — Chemnitz University of Technology, Institute of Physics, Germany

Since energy efficiency is becoming more and more important and novel nanostructured materials as well as new material groups have recently been introduced, the field of thermoelectricity is particularly in the focus of current research activities. One of the promising materials for future applications is $CoSb_3$ in its skutterudite phase. In this study, 30nm thick $CoSb_x$ films with different Sb content x have been deposited by MBE onto thermally oxidized Si(001) substrates. The deposition temperature was varied between room temperature and 300°C. In addition, samples deposited at room temperature have been annealed under UHV condition for one hour at different temperatures up to 700°C. The composition of these films was investigated by RBS and it was found that the Sb content of the deposited films is strongly dependant on the substrate temperature/annealing temperature. Structural investigations by XRD reveal the existence of the desired skutterudite phase in a narrow composition range and the influence of the preparation parameters on the phase formation will be discussed. In addition, the topography and electric conductivity was measured by AFM and four probe measurements, respectively. It was found that the morphology of the samples dominates the electrical conductance.

DS 13.6 Tue 11:45 H8

Doped NiTiSn as a n- + p-type thermoelectric material pair in almost one material — •B. Balke, S. Ouardi, M. Schwall, and C. Felser — Institute of Inorganic and Analytical Chemistry, Johannes Gutenberg - University, Mainz, Germany

Excellent n-type XNiSn (ZT_{max}=1.5) and p-type XCoSb ($ZT_{max} = 0.7$) (X = Ti, Zr, Hf) high temperature thermoelectrics were reported recently and reproduced by several groups in Asia (Toshiba, Toyota) and US. But to reach the goal to develop a thermoelectric converter (TEC) beyond the state-of-the-art for power generation one has to overcome several difficulties. The demands are environmental friendliness, low-cost and future availability of raw materials, high efficiency, operating temperature 100 - 700°C + short time excess temperature up to 800°C, possibility of industrial processing, and a thermoelectric material pair (n- + p-type) with very similar coefficients of thermal expansion and good thermoelectric compatibility. The half-Heusler materials class does meet nearly all requirements including a high power factor, but a general challenge in improving half-Heuslers is to reduce the comparatively high thermal conductivity. We produced and investigated the thermoelectric properties of doped NiTT'Sn(T = Ti, Zr, Hf, and T' = Sc, Y, V, Nb) and we were able to reach both goals, reducing the comparatively high thermal conductivity and designing a thermoelectric material pair (n- + p-type) in almost one material. *This work was financially supported by the Stiftung für Inovation Rheinland Pfalz.*

DS 13.7 Tue 12:00 H8

Enhanced Thermoelectric Figure of Merit in Edge Disordered Zigzag Graphene Nanoribbons — •Haldun Sevincli and Gianaurelio Cuniberti — Institute for Materials Science, TU Dresden, 01062 Dresden, Germany

We investigate electron and phonon transport through edge disordered zigzag graphene nanoribbons based on the same methodological tool of nonequilibrium Green functions [1]. We show that edge disorder dramatically reduces phonon thermal transport while being only weakly detrimental to electronic conduction. The behavior of the electronic and phononic elastic mean free paths points to the possibility of realizing an electron-crystal coexisting with a phonon-glass. The calculated thermoelectric figure of merit (ZT) values qualify zigzag graphene nanoribbons as a very promising material for thermoelectric applications.

[1] H. Sevincli and G. Cuniberti, arXiv:0908.3207

DS 13.8 Tue 12:15 H8

Calculation of the Seebeck-coefficient using the NEGF formalism in a 1D-model — •Michael Bachmann, Michael Czerner, and Christian Heiliger — I. Physikalisches Institut, Justus Liebig University Giessen, D-35392, Germany

We present a 1D model that can be used to calculate electron transport through interfaces of heterostructures. The model is based on the non-equilibrium Green's function (NEGF) formalism in the single band effective mass approximation. The effect of phonon scattering is taken into account by adding a self energy to the Hamiltonian. We obtain the Seebeck-coefficient within this model by applying a temperature difference and simultaneously adjusting the voltage to prevent a net current flow. The ratio of this voltage and the difference in temperature is the Seebeck-coefficient. We perform all calculations self consistently with respect to the Poisson equation. (SPP 1386)

DS 13.9 Tue 12:30 H8

Order-N method for calculating thermal transport at the mesoscale — •Wu Li[1,2], Haldun Sevincli[2], Stephan Roche[3,2], and Gianaurelio Cuniberti[2] — [1]Institute of Physics, Chinese Academy of Sciences, 100190 Beijing, China — [2]Institute for Materials Science and Max Bergmann Center of Biomaterials, Dresden University of Technology, 01062 Dresden, Germany — [3]CEA, Institute for Nanoscience and Cryogenics, INAC, SP2M, Lsim, 17 rue des Martyrs, 38054 Grenoble Cedex 9, France

We develop an order-N method for calculating the phonon transport in mesoscopic systems using the real space Kubo approach in the harmonic approximation. The advantage of our method over the Green function method is that we can compute the phonon transport properties of quasi-one dimensional structures as wide and as long as the experimentally relevant sample sizes within much shorter computation times. As a test case of this method, we calculate the elastic phonon mean free paths (MFP) of isotopically disordered carbon nanotubes (CNT). Our MFP values are in excellent agreement with the ones obtained from the Green function approach except for the very low energies. For such low energies, we use the analytic expression derived from perturbation theory. We apply the method to edge disordered graphene nanoribbons (GNR). We show that the phonon thermal conductance is reduced by more than two orders of magnitude due to edge disorder.

DS 13.10 Tue 12:45 H8

Strained and rolled up silicon: Electronic structure calculations of a promising thermoelectric material — •Nicki Hinsche, Bogdan Yavorski, Peter Zahn, and Ingrid Mertig — Martin-Luther-Universität, Institut für Physik, Von-Seckendorff-Platz 1, 06120 Halle/S.

Starting from bulk silicon, we studied the valley splitting due to symmetry breaking that occurs in rolled-up Si. Valley splitting in Si was studied recently because of tetragonal distortion and quantum well effects in heterostructures [1,2]. The new aspect in nowadays experimentally accessible rolled-up Si tubes is that symmetry breaking occurs in all spatial directions [3]. As a result, splitting of the six-fold degenerate conduction-band minimum is expected to be lifted. This has a strong influence on the transport properties as well. In detail, the anisotropy of the effective masses of charge carriers contributing to the conductivity in different directions will be studied in dependence on the applied strain. The electronic structure is calculated self consistently within the framework of density functional theory. The transport properties of the promising thermoelectric material will be studied in the diffusive limit of transport applying the Boltzmann theory in relaxation time approximation.

[1] Dziekan et al. Physical Review B 75, 195213 (2007) [2] Boykin et al. Physical Review B 70, 165325 (2004) [3] Cavallo et al. Journal of applied physics 103, 116103 (2008)

DS 14: Thermoelectric Thin Films and Nanostructures II

Time: Tuesday 14:00–15:30 Location: H8

Topical Talk DS 14.1 Tue 14:00 H8

Thermal Conductivity of Thermoelectric Materials Embedded with Nanoparticles — •Yee Kan Koh and David Cahill — Dept. of Materials Sc. and Eng., University of Illinois, Urbana, USA

Over the past decade, nanostructures are prevalently explored to reduce the thermal conductivity of existing thermoelectric materials and hence enhance the thermoelectric efficiency. In this regard, nanoparticles or nanodots embedded in a matrix could be effective in scattering phonons and thus reducing the thermal conductivity. We report here our thermal conductivity measurements of two important classes of thermoelectric materials, i.e., InAlGaAs embedded with ErAs nanoparticles and PbTe/PbSe nanodot superlattices (NDSLs). The samples are grown by our collaborators at UC Santa Barbara and MIT Lincoln Laboratory. We measured the thermal conductivity by time-domain thermoreflectance. From our measurements, we found that reduction of the thermal conductivity by ErAs nanoparticles is less significant in InAlGaAs than in InGaAs. By measuring TDTR in frequency domain, we showed that 3% of ErAs nanoparticles is sufficient to scatter phonons with mean-free-paths of 300-1000 nm. In contrast to InAlGaAs, we found that PbSe nanodots do not reduce the thermal conductivity of NDSLs below the alloy limits. All of our measurements approach the thermal conductivity of bulk homogenous alloys with the same average composition. We attribute this observation to short mean-free-paths of phonons in PbTe and small acoustic impedance mismatch between PbTe/PbSe. Our work provides guidelines for future work on thermoelectric materials embedded with nanoparticles.

DS 14.2 Tue 14:30 H8

Thermoelectric efficiency in stacks of n-type InAs/GaAs quantum dots — Vladimir M. Fomin[1] and •Peter Kratzer[2] — [1]Institut für Integrative Nanowissenschaften (IIN), Leibniz-Institut für Festkörper- und Werkstoffforschung (IFW) Dresden, D-01069, Dresden — [2]Fakultät für Physik und Center for Nanointegration (CeNiDE), Universität Duisburg-Essen, D-47048, Duisburg

We investigate the effect of the electron miniband energy spectrum of periodic 1D stacks of self-assembled InAs/GaAs quantum dots (QDs) with different geometrical parameters on their electronic transport employing the Boltzmann transport equation. The electron minibands are calculated within tight-binding and Kronig-Penney models. The transport relaxation time reveals a significant dispersion as a function of the wave vector in the stacking direction. The chemical potential is related to the concentration of electrons of the conduction band taking into account the minibands and a continuum. From the numerical analysis of the electric and thermal conductivities, the Seebeck coefficient and the figure-of-merit, we conclude that a 1D stack of QDs achieves a geometry-controlled enhanced efficiency as a thermoelectric converter in certain windows of the donor concentration. Reducing the QD height for a fixed stacking period is favourable for an increase of the figure-of-merit.

A fruitful collaboration with O. G. Schmidt and A. Rastelli and a financial support under the DFG SPP 1386 and the ESF Exchange Grant 2157 within the activity ‘Arrays of Quantum Dots and Josephson Junctions’ are gratefully acknowledged.

DS 14.3 Tue 14:45 H8

Thermal Conductivity Of Single Crystalline SiGe/Si Multilayers Below The Amorphous Limit — •Armando Rastelli, Fabio Pezzoli, Peixuan Chen, Mathieu Stoffel, and Oliver G. Schmidt — Institut für Integrative Nanowissenschaften, IFW Dresden, Helmholtzstr. 20, 01069 Dresden

We report on the fabrication, structural properties and cross-plane thermal conductivity measurements of multilayers of epitaxial SiGe self-assembled nanodots in Si matrix. Thermal conductivity measurements are performed with the differential 3-omega method using metal strips on top thin (30 nm thick) dielectric layers deposited by atomic layer deposition. With this approach we are able to reliably determine the cross-plane thermal conductivity of semiconductor layers as thin as 30 nm. Moreover we present a new method for error evaluation, which, based on Monte Carlo simulation, takes into account the uncertainties of all parameters entering in the model equations used to determine the thermal conductivity. The study reveals a rather linear dependence of the thermal conductivity on the SiGe interlayer spacing. For the thinnest Si-spacer thickness available (3 nm), our single-crystalline SiGe structure shows thermal conductivity values well below those of amorphous Si. Finally we discuss the results and possible routes to further reduce the thermal conductivity.

DS 14.4 Tue 15:00 H8

Half Heusler thin film superlattices for thermoelectrics — •Tino Jaeger[1], Christian Mix[1], Xenija Kozian[2], Benjamin Balke[2], Sascha Populoh[3], Anke Weidenkaff[3], Claudia Felser[2], and Gerhard Jakob[1] — [1]Institut für Physik, Universität Mainz, Staudinger ,Weg 7, 55099 Mainz, Germany — [2]Institut für Anorganische Chemie und Analytische Chemie, Universität Mainz, Staudinger Weg 7, 55099 Mainz, Germany — [3]EMPA - Eidgenössische Materialprüfung und -forschungs Anstalt Festkörperchemie und Katalyse, Ueberlandstrasse 129, 8600 Duebendorf, Switzerland

Due to rising energy costs and carbon dioxide concentration in the atmosphere interest on thermoelectric materials has strongly increased. The energy efficiency of thermoelectric devices has to be increased to expand the commercial usage. Here, efficiency is given by the figure of merit that is increased by a large Seebeck coefficient, large electrical conductivity and small thermal conductivity. Due to their electronic band structure half-Heusler alloys are appropriate candidates for such materials. Using thin film technology we prepare superlattices in order to increase the figure of merit. A superlattice based on NiTiSn and $NiZr_{0.5}Hf_{0.5}Sn$ is supposed to decrease the thermal conductivity due to phonon scattering at the interfaces. The epitaxial multilayer structures are synthesized by sputter technique in argon atmosphere.

A four-circle X-ray diffractometer allows the analysis of the crystal structures and the orientation of several layers with respect to each other. Resistivity, thermal conductivity and Seebeck coefficients are measured for different multilayers.

DS 14.5 Tue 15:15 H8

Engineering the thermopower in semiconductor-molecule junctions: towards high thermoelectric efficiency at the nanoscale — Daijiro Nozaki, Haldun Sevincli, Wu Li, •Rafael Gutierrez, and Gianaurelio Cuniberti — Institute for Materials Science and Max Bergmann Center of Biomaterials, Dresden University of Technology, D-01062 Dresden, Germany

We propose a possible route to achieve high thermoelectric efficiency in molecular junctions by combining a local chemical tuning of the molecular electronic states with the use of semiconducting electrodes. The former allows to control the position of the HOMO transmission resonance with respect to the Fermi energy while the latter fulfills a twofold purpose: the suppression of electronlike contributions to the thermopower and the cut-off of the HOMO transmission tails into the semiconductor band gap. As a result a large thermopower can be obtained. Our results strongly suggest that large figures of merit in such molecular junctions can be achieved [1].

[1] Engineering the thermopower in semiconductor-molecule junctions: towards high thermoelectric efficiency at the nanoscale, D. Nozaki, H. Sevincli, W. Li, R. Gutierrez, and G. Cuniberti, arxiv preprint: cond-mat 0908.0438 (2009).

DS 15: [HL] Organic Semiconductors: Transistors and OLEDs (Joint Session DS/CPP/HL/O)

Time: Tuesday 9:30–12:45 Location: H15

DS 15.1 Tue 9:30 H15

Ionic liquid gated polymer transistor — •Johannes Schöck, Daniel Secker, and Heiko B. Weber — Lehrstuhl für Angewandte Physik, Universität Erlangen-Nürnberg, Staudtstr. 7/A3, D-91058 Erlangen, Germany

We fabricate field-effect transistors with a polymer semiconductor using an ionic liquid top-gate, replacing the gate insulator. The geometry is bottom contact, liquid top gate. Electrical characterization yields a low conductance threshold of the device ($\sim -2.5\,\mathrm{V}$), and a steep increase of the source-drain current. An analysis points towards unusually high charge carrier mobility of the semi-conducting channel, with very favorable leakage currents through the gate. Strong hysteretic effects are observed.

DS 15.2 Tue 9:45 H15

Electrolyte-gated organic thin film transistors — •Felix Buth[1], Marin Steenackers[2], Deepu Kumar[1], Martin Stutzmann[1], and Jose Antonio Garrido[1] — [1]Walter Schottky Institut, Technische Universität München, Am Coulombwall 3, 85748 Garching, Germany — [2]Institute for Advanced Study, Technische Universität München, Arcisstr. 21, 80333 München, Germany

Organic semiconductors are today widely used as the active material in several applications based on thin film transistors. For most of these devices large operational voltages are required. One approach to reduce the gate voltage is increasing the capacitance of the gate dielectric. Several materials, including high-k dielectrics, ultra-thin cross-linked polymers or polyelectrolytes have been tested for this purpose. Among those, polyelectrolytes offer extraordinarily high capacitances with a relatively low technology cost. The high capacitance results from the electrical double layer formed at the polyelectrolyte/semiconductor interface, opening the possibility of using organic thin film transistors for biological and chemical sensors, in which in-electrolyte operation is required. Since, however, water stable organic semiconductors are generally deposited by evaporation in UHV, the surface of the polyelectrolyte needs to be smooth to enable the growth of high quality films. In this contribution the properties of different polyelectrolyte dielectrics are investigated. We show how polyelectrolytes can be directly prepared on conductive substrates, resulting in homogeneous films with high interfacial capacitances. Furthermore, we show the preparation of high quality pentacene thin films onto the polyelectrolyte films.

DS 15.3 Tue 10:00 H15

Molecular weight dependent short channel effect in MDMO-PPV — •Ali Veysel Tunc, Elizabeth von Hauff, and Jürgen Parisi — University of Oldenburg, Department of Physics, Energy and Semiconductor Research Laboratory, Carl-von-Ossietzky Str. 9-11, 26129 Oldenburg, Germany

In this study, organic field effect transistors (OFETs) based on poly [2-methoxy,5-(3',7'-dimethyl-octyloxy)]-p-phenylene vinylene (MDMO-PPV) with two different weight-average molecular weights (Mw) were fabricated and the effect of the molecular weight on the device properties was investigated. It was observed that the operation performance of the OFET depends on the molecular weight and channel length. The short channel effect was observed, i.e. a lack of saturation in the output characteristic with a fixed gate voltage. We found that the saturation behavior and hole mobility of a given material strongly depend on molecular weight. Short channel effects were observed in higher molecular weight for MDMO-PPV. The hole mobility around 10 times better for higher molecular weight that has been shown in literature.

DS 15.4 Tue 10:15 H15

Electron Mobility in Methanofullerens — •Maria S Hammer[1], Carsten Deibel[1], and Vladimir Dyakonov[1,2] — [1]Experimental Physics VI, Julius-Maximilians-University of Würzburg, Am Hubland, D-97074 W\"urzburg — [2]ZAE Bayern, Div. Functional Materials for Energy Technology, Am Hubland, D-97074 Würzburg

Methanofullerenes are the state of the art acceptor-type semiconductors applied in flexible and printed electronic devices, e.g. they are used together with a donor-type polymer in (i) solar cells or (ii) complementary circuits. While the hole transport in polymers has been intensely investigated within the last years, less attention has been drawn to the fundamentals of the transport within methanofullerenes. In the present study, the electron mobility, which strongly depends on the electron density, is investigated.

We utilize the organic field effect transistor (OFET) as it provides a way of probing the mobility within a wide range of electron densities via gate voltage. Nevertheless, the performance of an OFET sensitively depends on electron injection from the contacts and trapping at the dielectric interface. Therefore, in order to assess the transport parameters of methanofullerenes, it is indispensable to vary the work function of the electrodes as well as the insulator. We will investigate and discuss the ambipolar charge transport in dependence of the charge carrier density in [6,6]-phenyl-C61-butyric acid methyl ester and other derivatives, employing a variation of dielectric surfaces and injecting metals.

DS 15.5 Tue 10:30 H15

Correlation between the effective contact resistance and the charge carrier transport in organic semiconductors of different mobility — R. Winter[1], F. Wörner[1], M.S. Hammer[1], C. Deibel[1], and •J. Pflaum[1,2] — [1]Experimental Physics VI, Julius-Maximilians-University, 97074 Würzburg — [2]Bavarian Center For Applied Energy Research, 97074 Würzburg

In this presentation we address questions on the impact of the charge carrier mobility on the injection behavior in organic thin film transistors (OTFTs). Though many theoretical models treat the contact resistance, R, and the mobility, μ, independently, we demonstrate a significant correlation between these two quantities for P3HT and pentacene. Corresponding TFT measurements have been performed between 40 - 300K. To modify the effective contact resistance, monolayers of different oligoacenes were deposited between the Au bottom contacts and the active organic transport layer. Despite significant differences in the room temperature mobilities, $10^{-4}\mathrm{cm}^2/\mathrm{Vs}$ for P3HT and $10^{-2}\mathrm{cm}^2/\mathrm{Vs}$ for pentacene, the temperature dependent variations of the mobility as well as of the effective contact resistance prove to be similar. For both materials a change in the slope of the R(T) and μ(T)-slope can be detected. However, the cross-over temperature for pentacene amounts to 80K whereas that for P3HT is shifted to 185K. We will discuss this observation in the context of a balanced transport, i.e. that the injection at the metal contact interfaces is strongly related to the charge carrier transport in the semiconducting layer.

Financial support by BMBF (project GREKOS) is acknowledged.

DS 15.6 Tue 10:45 H15

Thickness dependence of contact and sheet resistance of thiophene and pentacene based organic field effect transistors — •Torsten Balster, Steve Pittner, Dagmawi Belaineh, Arne Hoppe, and Veit Wagner — School of Engineering and Science, Campus Ring 1, Jacobs University Bremen, 28759 Bremen, Germany

The electrical properties of evaporated organic semiconductors in dependence on the film thickness are affected by the growth mode of the thin film. While dihexyl-substituted oligothiophenes (DHnT) show a typical layer-by-layer growth mode on hexamethyldisilazane(HMDS)-treated silicon oxide, pentacene exhibits 3-dimensional growth. The growth mode as determined by AFM investigations is also reflected in the integral in-situ IV-measurements during growth. DHnT shows oscillatory behaviour in the mobility and the contact resistance within the first two monolayers, whereas the pentacene saturates without oscillations for 10nm. The total contact resistance with gold electrodes has been evaluated by the transfer line method. Furthermore the potential barriers at source and drain contact are determined separately by a four probe setup. For this purpose, additional sense fingers are prepared within the channel allowing the direct access to the channel potential. Major contact effects are identified for channel length smaller than 10 microns.

DS 15.7 Tue 11:00 H15

Semiconducting Thin Films of Fluorinated and Unsubstituted Phthalocyanines for Applications in Organic Field Effect Transistors — •Harry Brinkmann[1], Christopher Keil[1], Olga Tsaryova[2], Dieter Wöhrle[2], and Derck Schlettwein[1] — [1]Institute of Applied Physics, Justus-Liebig-University Giessen, Germany. email:schlettwein@uni-giessen.de — [2]Institute of Organic and Macromolecular Chemistry, University of Bremen, Germany.

Perfluorinated phthalocyanines ($F_{16}Pc$) show n-type characteristics as active layers in organic field transistors while organic field transistors with unsubstituted phthalocyanines (Pc) exhibit p-type characteristics. The growth of $F_{16}Pc$ and Pc films has been studied in OFETs on organic (polyimide, $PMMA$) and inorganic insulating layers (SiO_2) with different surface modifications ($HMDS$ treatments). We report here about the dependence of the growth mode of the films and the field effect mobility on the used substrate for the copper complexes. The development of the electrical conduction was studied in-situ during film growth and the field effect mobility was determined for various film thicknesses in different regimes of the Stranski-Krastanov growth mechanism that led to the formation of ultrathin conductive layers in the monolayer range followed by reorganization towards island growth. Optical absorbance was measured in reflection or transmission in dependence of the used substrate to investigate details of the intermolecular coupling.

15 Min. Coffee Break

DS 15.8 Tue 11:30 H15

Carrier density in a Gaussian density of states: Approximation for the Gauss- Fermi integral — •Gernot Paasch[1] and Susanne Scheinert[2] — [1]IFW Dresden — [2]TU Ilmenau

The density of hopping transport states in organics can be approximated by a Gaussian DOS. As a consequence, the mobility becomes a function of carrier density, field and of course temperature. Such dependencies can now be implemented easily in advanced device simulation programs as Sentaurus Device. However, the carrier density as function of the Fermi energy is not taken into account until now. For inorganic semiconductors with a square root DOS the situation was similar with the carrier density expressed by the Fermi- Dirac integral F1/2. Further Fermi-Dirac integrals are needed for the electronic energy density and for Einstein's relation. For these cases analytical approximations have been developed early allowing for fast simulation. For the Gaussian DOS the carrier density is given by the integral over the product of Gaussian DOS and Fermi-Dirac distribution, the Gauss-Fermi integral. Related integrals describe the electronic energy density and occur in Einstein's relation. Here we present an extremely simple and accurate approximation for the Gauss-Fermi integral and discuss its potential applicability in simulation of organic devices.

DS 15.9 Tue 11:45 H15

Comparative transport studies in Bridgman and sublimation grown 9,10-Diphenylanthracene single crystals. — •Andreas Steindamm[1], Ashutosh K. Tripathi[2], Rainer Stöhr[3], Jörg Wrachtrup[3], and Jens Pflaum[1] — [1]Institute of Experimental Physics VI, Julius-Maximilians-University, 97074 Würzburg, Germany — [2]Holst Centre/TNO, 5656 AE Eindhoven, NL — [3]Physikalisches Institut, University of Stuttgart, 70550 Stuttgart, Germany

To improve organic electronic applications, knowledge about microscopic mechanisms determining the charge carrier mobilities is pivotal. 9,10-Diphenylanthracene (DPA) has been identified as model system to study those correlations due to its high electron and hole mobilities at room temperature [1] and its complex structural phase behaviour. We will demonstrate our temperature dependent Time-Of-Flight data on single crystals grown by vapor phase transport (VPT) and by Bridgman growth technique. Both preparation techniques revealed crystals of different morphologies resulting in significant variations of the related bipolar mobilities. As a key result, the charge carrier mobility of $\sim 1 cm^2/Vs$ at room temperature along the (111)-direction of Bridgman crystals exceeds that along the (001)-direction of VPT grown crystals by about one order of magnitude. The observed differences in the mobility data will be discussed in the context of the microscopic molecular arrangement within the respective crystal structure. Financial support by BMBF (project GREKOS) is acknowledged.

[1] Tripathi A. K. et al., Adv. Mater. 19 (2007) 2097

DS 15.10 Tue 12:00 H15

Probing charge carrier dynamics in conducting polymers using single molecules as sensors — •Maximilian Nothaft[1], Steffen Höhla[2], Aurélien Nicolet[3], Jens Pflaum[4], Fedor Jelezko[1], and Jörg Wrachtrup[1] — [1]3. Phys. Ins., Univ. Stuttgart — [2]Chair of Display Technology, Univ. Stuttgart — [3]MoNOS, Huygens Laboratory Leiden — [4]Exp. Phys. VI, Univ. Wuerzburg and ZAE Bayern

Doping of conducting polymers by guest molecules is widely applied in organic light emitting devices to improve their efficiency. By reducing the concentration of suited guest molecules it becomes possible to study the dynamics of single molecule emitters using confocal microscopy.

In our contribution we discuss the optical properties of single Dibenzoterrylene dye molecules dispersed in an OLED consisting of PPV as host material. It will be shown how to prepare devices of photostable single molecules in PPV emitting a constant flux of single photons at room temperature by excitation from a Ti:sapphire laser.

By simultaneous laser excitation and electrical operation it is possible to detect the effect of injected charge carriers on the dynamics of single quantum emitters. Since the ratio of singlet to triplet exciton formation in the device is 1:3, this leads to an effective pumping to the triplet state of the single molecule thereby reducing its fluorescence intensity. Modeling this process it becomes possible to associate the reduced fluorescence intensity with the local current density at the position of the molecule. This correlation enables us to optically probe the current density in an OLED with nm spatial resolution.

DS 15.11 Tue 12:15 H15

Energy band alignment at the oxide-organic interface ITO/ZnPC determined by photoelectron spectroscopy — •Jürgen Gassmann and Andreas Klein — Surface Science Department, Istitute of Materials Science, TU Darmstadt, Germany

The possibility to generate light on the front- and backside of an organic light-emitting diode (OLED) is given for inverted top-emitting OLEDs. For them the transparency of the back contact is crucial. Here transparent conductive oxides (TCO) like indium tin oxide (ITO) or zinc oxide are of special interest, because these films can be deposited with magnetron sputtering at room temperature. In this work the energy band alignment between the organic material zinc phthanalocyanine (ZnPC) and the transparent oxide ITO is evaluated. For this the X-ray photoelectron spectroscopy technique (XPS) is used and combined with an in-situ preparation of the films. The energy band alignments of the deposition sequences ITO on ZnPC and vice versa are compared. Here valence band offsets up to 1.3eV can be detected. The energy band alignment shows a strong dependence on the deposition sequence. Additionally the electrical and optical properties of ITO films sputtered at room temperature are investigated.

DS 15.12 Tue 12:30 H15

Highly efficient white top-emitting organic light-emitting diodes with forward directed light emission — •Patricia Freitag, Sebastian Reineke, Mauro Furno, Björn Lüssem, and Karl Leo — Institut für Angewandte Photophysik, TU Dresden, George-Bähr-Straße 1, 01069 Dresden, Germany

The demand for highly efficient and energy saving illumination has increased considerably during the last decades. Organic light emitting diodes (OLEDs) are promising candidates for future lighting technologies. They offer high efficiency along with excellent color quality, allowing substantially lower power consumption than traditional illuminants. Recently, especially top-emitting devices have attracted high interest due to their compatibility with opaque substrates like metal sheets. In this contribution, we demonstrate top-emitting OLEDs with white emission spectra employing a multilayer hybrid cavity structure with two highly efficient phosphorescent emitter materials for orange-red (Ir(MDQ)2(acac)) and green (Ir(ppy)3) emission as well as the stable fluorescent blue emitter TBPe. To improve the OLED performance and modify the color quality, two different electron blocking layers and anode material combinations are tested. Compared to Lambertian emission, our devices show considerably enhanced forward emission, which is preferred for most lighting applications. Besides broadband emission and angle independent emission maxima, power efficiencies of 13.3 lm/W at 3 V and external quantum efficiencies of 5.3% are achieved. The emission shows excellent CIE coordinates of (0.420, 0.407) at approx. 1000 cd/m2 and color rendering indices up to 77.

DS 16: [CPP] Organic Electronics and Photovoltaics I (Joint Session DS/CPP/HL/O)

Time: Tuesday 9:30–12:45 Location: H37

DS 16.1 Tue 9:30 H37

Side chain variations on dicyanovinyl-oligothiophenes studied by photoinduced absorption spectroscopy: consequences for small molecule organic solar cells — •Hannah Ziehlke[1], Roland Fitzner[2], Christian Koerner[1], Egon Reinold[2], Peter Baeuerle[2], Karl Leo[1], and Moritz Riede[1] — [1]Institut für Angewandte Photophysik, Technische Universität Dresden — [2]Institut für Organische Chemie II und Neue Materialien, Universität Ulm

Oligothiophenes capped with electron-withdrawing dicyanovinyl groups (DCVnT) are promising candidates for applications in small molecule organic solar cells. These oligothiophene derivatives can act as electron donor in blend layers with C_{60}. Single heterojunction devices reach efficiencies above 4 %. The introduction of side chains as intermolecular spacer has little effect on the energetics and mainly influences the morphology of the evaporated thin film. In addition, the distance between donor and acceptor molecules and thus the energy transfer and charge separation at the interface can be controlled. The energetic and dynamic properties of the long lived photoexcitations in pristine and blend layers can be obtained by photoinduced absorption spectroscopy (PIA). We here characterize of DCV3T with zero, two, and four alkyl chains (Methyl and Butyl) via PIA spectroscopy complemented with morphological studies. Our results indicate that the energy transfer process at the heterojunction is more efficient for smaller spatial distances between donor and acceptor molecules.

DS 16.2 Tue 9:45 H37

New multiwall molecular organic nanotubes — •Maren Rastedt[1], Frauke Kutscher[1], Okko Frey[2], Rüdiger Beckhaus[2], Christian Maibohm[3], and Katharina Al-Shamery[1] — [1]University of Oldenburg, Physical Chemistry 1, Germany — [2]University of Oldenburg, Inorganic Chemistry, Germany — [3]NanoSYD, Sonderborg, Denmark

Nanotubes can be described as the newest star in the evening sky of nanotechnology. Since the discovery of carbon nanotubes , this nanostructure has grasped the mind of many. This structure has many application possibilities ranging from liquid and gas storage to microelectronics and sub wavelength optical components and fibers. In our presentation we will give an introduction to multiwall nanotubes made from Tetrabenzofluorene(Tbf)-derivates. These Tbf-nanotubes have attracted interest because of their many properties, e.g. crystallization and waveguiding. Our nanotubes are prepared by the elegant and simple process of template assisted assembly. The assembly process will be presented together with specific properties of different Tbf-nanotubes. By changing growth parameters in the assembly process we have a method for probing fundamental questions and properties of our nanotubes. One future application of our nanotubes could be as an active element in a photovoltaic device.

DS 16.3 Tue 10:00 H37

Radical Molecular Wires — •Georg Heimel[1], Egbert Zojer[2], Lorenz Romaner[3], Jean-Luc Brédas[4], and Francesco Stellacci[5] — [1]Institut für Physik, Humboldt-Universität zu Berlin, Germany — [2]Institut of Solid State Physics, Graz University of Technology, Austria — [3]Chair of Atomistic Modeling and Design of Materials, University of Leoben, Austria — [4]School of Chemistry and Biochemistry, Georgia Institute of Technology, Atlanta, USA — [5]Department of Materials Science and Engineering, Massachusetts Institute of Technology, Cambridge, USA

The technological relevance and the functionality of semiconducting materials originate in the fact that their conductivity and the band alignment at the interfaces with other materials can be controlled through doping. Here, we consider the ultimate miniaturization of functional devices by computationally investigating the doping of molecular wires suspended between two metal electrodes.[1] For representative systems we find that, upon doping, the molecular conductivity is enhanced by more than two orders of magnitude. We elucidate the microscopic origin of this dramatic effect and present an intuitive picture, which rationalizes our observations in terms of *Fermi-level pinning*. Our results shed new light on recent experimental findings and, most importantly, in-depth understanding of the doping mechanism enables the targeted development of new functional components for sensing and switching at the single-molecule scale.

[1] G. Heimel et al., *Nano Lett.* **9**, 2559 (2009).

DS 16.4 Tue 10:15 H37

Structure property relationship in aza-bodipy absorber materials for organic photovoltaics — •Roland Gresser, Toni Mueller, Moritz Philipp Hein, Karl Leo, and Moritz Riede — Institute of Applied Photophysics, Dresden University of Technology, Germany

In this joint experimental and theoretical study, we focus on the structure property relationship of aza-bodipy dyes as active donor materials in vacuum deposited small molecule solar cells.

The position of the materials HOMO can be intentionally varied by the choice of the functional group attached to the molecule. The absorption spectra show a red shift of the maximum with increasing donor strength of the substituents due to the increasing HOMO energy and decreasing band gap.

Based on crystal structure data, the charge carrier mobility determining parameters like reorganization energies and transfer integrals are calculated. The results show an increasing molecular orbital overlap and significant higher transfer integrals upon planarization and rigidification of the molecule. With this information, the observed charge carrier mobility differences from experiment can be explained.

In addition to the electronic properties a high thermal and photo stability is essential. From combined thermogravimetric analysis and mass spectroscopy we could determine the degradation process of the material and were able to increase the thermal stability by substitution of the involved species.

DS 16.5 Tue 10:30 H37

Dicyanovinyl sexithiophenes: self-organization and photovoltaic properties — •Marieta Levichkova[1], David Wynands[1], Alexandr Levin[1], Karl Leo[1], Karsten Walzer[2], Dirk Hildebrandt[2], Peter Bäuerle[3], Rosina Rentenberger[4], and Moritz Riede[1] — [1]Institut für Angewandte Photophysik, TU Dresden, Germany — [2]Heliatek GmbH, Dresden, Germany — [3]Institut für Organische Chemie II und Neue Materialien, Universität Ulm, Germany — [4]Institut für Physik, TU Ilmenau, Germany

Recently, vacuum deposited films consisting of conjugated dicyanovinyl-capped (DCV) oligothiophenes have shown significant potential as photoactive layers in small molecule solar cells [1]. Here, we study the structural and optical properties of films of two DCV-derivatives both comprising six thiophene rings (DCV6Ts) but having different side groups. For both derivatives, neat DCV6T and mixed

DCV6T:C60 films are compared using UV-VIS absorption and photoluminescence spectroscopy, X-ray diffraction (XRD), and Atomic Force Microscopy. It is shown that the modification of the molecular structure results in a structured and red shifted absorption band, which indicates better molecular arrangement in the solid state. The improved self-organization at room temperature deposition is confirmed by XRD. Furthermore, the nanomorphology of the mixed DCV6T:C60 films is optimized using substrate heating. Bulk heterojunction solar cells with power conversion efficiencies exceeding 4% are presented.

[1] K. Schulze et al., Adv. Mater. 2006, 18, 2872-2875

15 min. break

DS 16.6 Tue 11:00 H37

Hexaazatriphenylene and hexaazatrinaphthylene derivatives as electron transport materials in organic solar cells — •Christiane Falkenberg[1], Martin Baumgarten[2], Ralph Rieger[2], Selina Olthof[1], Karl Leo[1], Moritz Riede[1], and Klaus Müllen[2] — [1]Institut für Angewandte Photophysik, TU Dresden, 01069 Dresden — [2]MPI für Polymerforschung, 55128 Mainz

There is increasing interest in molecularly doped organic materials for the fabrication of efficient organic electronic devices. In small molecule organic solar cells, the so-called p-i-n concept is advantageous for the independent optimization of electrical and optical properties. Here, the absorbing donor-acceptor heterojunction is sandwiched between a p-doped hole transport layer and an n-doped electron transport layer. The design of suitable functional molecules for the transport layers is currently an important issue, however, the choice of available wide-gap materials for the n-side of organic solar cells is very limited. Here, we investigate hexaazatriphenylene and hexaazatrinaphthylene derivatives as substitutes for the common electron transport materials C_{60} or BPhen and BCP. Having bandgaps of > 2.7eV the new materials are transparent which, in combination with a suitable position of the energy levels, enables exciton blocking. Furthermore molecular doping with either acridine orange base (AOB) or NDN1 (Novaled AG) leads to an increase of the conductivity by several orders of magnitude, reaching values beyond $1{\cdot}10^{-6}$ S/cm. Altogether the beneficial optical and electrical properties allow the fabrication of organic solar cells with increased efficiency compared to the standard devices.

DS 16.7 Tue 11:15 H37

Structure - property relationship of thiophene based materials bearing different accepting groups — •Marion Wrackmeyer, Markus Hummert, Horst Hartmann, Karl Leo, and Moritz Riede — Institut für Angewandte Photophysik, Technische Universität Dresden, Germany

Organic solar cells require new materials for improved efficiencies. The relationship of molecular structure and properties is very important to optimise the devices. An interesting class of materials are thiophene block co-oligomers. The materials obtain electron donating (D) and accepting (A) groups and have the general structure A-D-A or D-A-D. In particular, the investigation of electron accepting groups is very important, because they have a high influence on the electronic structure of an organic molecule and are therefore an influential impact in the performance of a small molecule p-i-n solar cell. We present investigations on thiophene based materials bearing different accepting groups. The accepting groups are eg dicyanovinyl, dioxaborine, and benzthiadiazole. The materials were synthesised by Stille-coupling. Basic precondition for all materials is the thermal stability for deposition by vacuum-techniques. Subsequent investigations focus on absorption (solution and thin films), electrochemical behaviour (cyclic voltammetry to investigate the frontier molecular orbital energy levels), DFT-calculations (to show the location of HOMO and LUMO), mobility, morphology, dopability, and the properties of a solar cell.

DS 16.8 Tue 11:30 H37

Charge transport in self-assembled semiconducting organic layers: role of dynamic and static disorder — •Thorsten Vehoff[1], Yeon Sook Chung[2], Karen Johnston[1], Alessandro Troisi[3], Do Yeung Yoon[2], and Denis Andrienko[1] — [1]Max Planck Institut fuer Polymerforschung, Ackermannweg 10, 55128 Mainz, Germany — [2]Department of Chemistry, Seoul National University, Seoul 151-747, Republic of Korea — [3]Department of Chemistry and Centre of Scientific Computing, University of Warwick, Coventry, CV4 7AL, United Kingdom

Partial disorder is an inherent property of self-assembled organic semiconductors that complicates their rational design, since electronic structure, self-assembling properties and stability all have to be accounted for simultaneously. Therefore, the understanding of charge transport mechanisms in these systems is still in its infancy. A theoretical study of charge transport in organic semiconductors was performed on self-assembled layers of [1]Benzothieno[3,2-b]benzothiophene functionalized with alkyl side chains. Analysis showed that semiclassical dynamics misses static (on timescales of charge transport) disorder while the solution of the master equation combined with the high-temperature limit Marcus theory for charge transfer rates does not take into account molecular dynamic modes relaxing on a timescale of charge hopping. A comparison between predictions based on a perfectly ordered and a realistic crystal structure reveals the strong influence of static and dynamic disorder. The advantage of two-dimensional charge transporting materials over one-dimensional ones is clearly shown.

DS 16.9 Tue 11:45 H37

Charge Transport in rr-P3HT:PCBM Blends - The Impact of Ultrahigh Regioregularity on Hole Transport and Device Performance — •Ralf Mauer and Frédéric Laquai — Max-Planck-Institut für Polymerforschung, Mainz, Deutschland

Blends of poly(3-hexylthiophene) (P3HT) and [6,6]-phenyl C_{61} butyric acid methyl ester (PCBM) have emerged as a prototypical material system for bulk heterojunction solar cells with reasonable efficiencies during the past five years. Despite tremendous engineering efforts to push devices to 5% power conversion efficiency (PCE), the correlation between charge carrier mobility and device performance is still up for debate. Theoretical models range from "the higher - the better" over optimum finite mobilities to no effect of mobility on PCE at all.

We investigate charge transport in pristine P3HT films and in blends with PCBM by the time of flight (TOF) technique and analyse the results in the framework of the Gaussian disorder model. In order to understand the effect of charge transport on solar cell efficiency, we examine P3HT with three different regioregularities, i.e. regiorandom P3HT, rr-P3HT with high (rr=94%) and with ultrahigh (rr>98%) regioregularity. While the regioregularity is known to have a strong influence on the charge carrier mobility, its effect on other transport parameters, especially on the energetic disorder of hole transport in P3HT, is reported by us for the first time.

Finally, we correlate the TOF results and spectroscopic measurements with device performance to determine the influence of charge transport on the power conversion efficiency.

DS 16.10 Tue 12:00 H37

Charge transport in conjugated polymers with energetic disorder — •James C Blakesley[1,2], Helen S Clubb[1], Christopher Groves[1], Louise M Hopkins[1], and Neil C Greenham[1] — [1]University of Cambridge, Cambridge, UK — [2]Universität Potsdam, Potsdam, Germany

We investigate charge transport in sandwich-type devices with two polyfluorene-based copolymers: poly(9,9-dioctylfluorene-co-bis(N,N'-(4,butylphenyl))bis(N,N'-phenyl-1,4-phenylene)diamine) (PFB) and poly(9,9-dioctylfluorene-co-benzothiadiazole) (F8BT). A standard analysis of the data produces a poor fit to the data, with an apparent dependence of mobility on device thickness. Previously, such behaviour in electron transport has been attributed to trapping[1]. However, we find that a good fit is obtained by using a numerical simulation based on energetic disorder that takes into account the effects of electric field and carrier density on mobility (Extended Gaussian Disorder model). The amount of energetic disorder is quantified by 110+/-10meV and 100+/-10meV respectively. When the two materials are blended together, hole mobility remains constant when the fraction of PFB is 50% or greater, but drops dramatically for low concentrations of PFB. The amount of energetic disorder remains unaffected by any degree of blending, suggesting that there is no change in microscopic ordering of the polymers upon blending.

[1] R. Steyrleuthner, S. Bange and D. Neher, J. Appl. Phys. 105, 064509 (2009)

DS 16.11 Tue 12:15 H37

Towards high charge carrier mobilities by rational design of organic semiconductors — •Denis Andrienko[1], Valentina Marcon[2], James Kirkpatrick[3], Victor Ruehle[1], Bjoern Baumeier[1], Thorsten Vehoff[1], Alexander Lukyanov[1], Kurt Kremer[1], Jenny Nelson[3], and Christian Lennartz[4] — [1]Max Planck Institute for Polymer Research, Mainz — [2]Technische Universität Darmstadt, Germany — [3]Imperial College London, UK — [4]BASF AG, Ludwigshafen

The role of material morphology on charge carrier mobility in partially disordered organic semiconductors is discussed for several classes of materials: derivatives of hexabenzocoronenens [1], perylenediimides [2], triangularly-shaped polyaromatic hydrocarbons [3], and Alq3. Simulations are performed using a package developed by Imperial College, London and Max Planck Institute for Polymer Research, Mainz (votca.org). This package combines several techniques into one scheme: quantum chemical methods for the calculation of molecular electronic structures and reorganization energies; molecular dynamics and systematic coarse-graining approaches for simulation of self-assembly and relative positions and orientations of molecules on large scales; kinetic Monte Carlo and master equation for studies of charge transport.

[1] J. Kirkpatrick, et al, Phys. Rev. Lett., 98, 227402, 2007; [2] V. Marcon, et al, J. Am. Chem. Soc., 131, 11426, 2009; [3] X. Feng et al, Nature Materials 8, 421, 2009

DS 16.12 Tue 12:30 H37

Fully functionalized block copolymers for organic electronic applications — •Sven Hüttner[1,2], Michael Sommer[2], Justin Hodgkiss[1], Peter Kohn[3], Thomas Thurn-Albrecht[3], Richard Friend[1], Ullrich Steiner[1], and Mukundan Thelakkat[2] — [1]Cavendish Laboratory, University of Cambridge — [2]Angewandte Funktionspolymere, Makromolekulare Chemie I, Universität Bayreuth — [3]Experimentelle Polymerphysik, Universität Halle-Wittenberg

Block copolymers are well known to phase separate in highly ordered nanostructures on length scales commensurate with the exciton diffusion length. We use fully functionalized block copolymers for photovoltaic devices, where a donor and an acceptor polymer are covalently linked. The acceptor block consists of a polyacrylate backbone with pendant perylene bisimide moieties and the donor block consists of poly(3-hexylthiophene) (P3HT). We combine temperature dependent small angle and wide-angle X-ray scattering measurements to investigate the block copolymer phase separation as well as the influence of the crystallisation kinetics of the two blocks. Intermolecular and intramolecular interactions drive the self-assembly of structures from molecular lengthscales to larger mesostructures of some nanometers to microphase separation of some tens of nanometers. The investigation of the morphology is accompanied by steady state spectroscopy and transient absorption spectroscopy. Furthermore organic thin film transistors are used to characterize the transport properties in these novel materials which are found to exhibit unique properties such as the tunability between n-type, p-type or ambipolar transport.

DS 17: [CPP] Organic Electronics and Photovoltaics II (Joint Session DS/CPP/HL/O)

Time: Tuesday 13:45–16:15 Location: H37

DS 17.1 Tue 13:45 H37

Spectroscopic signatures of C_{70}-Anions in Polymer-Fullerene composites — •Andreas Sperlich[1], Moritz Liedtke[2], Hannes Kraus[1], Oleg Poluektov[4], Carsten Deibel[1], Nazario Martin[3], and Vladimir Dyakonov[1,2] — [1]Experimental Physics VI, Physical Institute, Julius-Maximilians-University of Würzburg, D-97074 Würzburg — [2]ZAE Bayern, Div. Functional Materials for Energy Technology, D-97074 Würzburg — [3]Departamento de Quimica Organica, Facultad de Quimica, Universidad Complutense, E-28040 Madrid — [4]Chemical Sciences and Engineering Division, Argonne National Laboratory, 9700, USA

C_{70}-derivates are used in the most efficient organic bulk heterojunction solar cells. However, the detailed photophysical processes in composites containing C_{70} are still unresolved. In this contribution, our focus is on the light-induced charge transfer from the polymer to the fullerene, generating negatively charged C_{70} radicals. Photoinduced absorption (PIA), electron spin resonance (ESR 9.5GHz) and optically detected magnetic resonance (ODMR) were used to draw a picture of the photoinduced charge transfer from polymers to C_{70}. We provide the first experimental identification of the light induced C_{70} radical anion in blends with P3HT using high frequency ESR (130GHz). Comparing spectra from C_{70}-derivates with different sidechains, we could confirm that the electron is indeed localized on the C_{70}-cage. Further, we identify an additional absorption band at 0.9eV due to C_{70}^- by PIA.

DS 17.2 Tue 14:00 H37

The Localized Nature of Charge Transfer in F_4TCNQ-Doped Thiophene-Based Donor Polymers — •Patrick Pingel[1], Lingyun Zhu[2], Kue Surk Park[1], Jörn-Oliver Vogel[1], Silvia Janietz[3], Eung-Gun Kim[2], Jürgen P. Rabe[1], Jean-Luc Brédas[2], and Norbert Koch[1] — [1]Department of Physics, Humboldt University Berlin, Germany — [2]School of Chemistry and Biochemistry, and Center for Organic Photonics and Electronics, Georgia Institute of Technology, USA — [3]Fraunhofer IAP, Potsdam, Germany

Recently, polymer layers exhibited exceptionally high conductivities upon p-type doping with the molecular acceptor tetrafluorotetracyanoquinodimethane (F_4TCNQ). Here, we present experimental and theoretical results on blend layers of F_4TCNQ and a series of poly(3-hexylthiophene-*co*-dithienyltetrafluorobenzene) (P3HT-TFT) copolymers with systematically varied TFT content. Regardless of the amount of TFT in the donor polymer, we find that only a single charge transfer (CT) species is formed, which we assign to the interaction of F_4TCNQ with an oligothiophene segment of the main chain. The degree of CT remains constant, even if the dopant concentration is increased up to a point, where closely neighbouring CT complexes exist at the same uninterrupted thiophene segment. Our findings show that the CT between F_4TCNQ and an oligothiophene segment has a localized, isolated nature, possibly comprising less than five connected thiophene units. Thus, CT is dictated by the local electronic structure on the nm scale, rather than depending, e.g., on the macroscopic ionization potential determined from photoemission methods.

DS 17.3 Tue 14:15 H37

Charge Transfer Exciton Dynamics in Polymer/Fullerene Blend — •Josef M. Berger, Markus Hallermann, Enrico Da Como, and Jochen Feldmann — Lehrstuhl für Photonik und Optoelektronik, CeNS, LMU München

Polymer fullerene blends are one of the most promising material systems for organic photovoltaics. A major loss channel in these cells is the formation and recombination of charge transfer excitons. These excitons emit light as a consequence of radiative recombination of the hole on the polymer and the electron on the fullerene [1]. Here, we report on time resolved emission experiments with the aim of understanding the parameters controlling the recombination lifetime. For the blend of MDMO-PPV/PCBM we correlate the decay profile with the morphology obtained by transmission electron microscopy [2]. [1] Markus Hallermann, Stephan Haneder, and Enrico Da Como, Appl. Phys. Lett 93, 053307 (2008) [2] Markus Hallermann, Ilka Kriegel, Enrico Da Como, Josef M. Berger, Elizabeth von Hauff, Jochen Feldmann, Advanced Functional Materials 19, 3662 (2009)

DS 17.4 Tue 14:30 H37

The Relationship between the Electric Field Induced Dissociation of Charge Transfer (CT) Excitons and the Photocurrent in Novel Hybrid Small Molecular/Polymeric Solar Cells — •Sahika Inal[1], Alan Sellinger[2], and Dieter Neher[1] — [1]Universität Potsdam, Institut für Physik und Astronomie, 14476 Potsdam-Golm — [2]Institute of Materials Research & Engineering, Singapore 117602

Complete dissociation of coulombically bound interfacial states is an ultimate step accounting for photovoltaic performance. Recent work has proposed that the emission of CT-exciton, i.e. an exciplex, is a competing process to the generation of free charges [Appl. Phys. Lett. 2007, 90, 092117]. Here, we investigated the photophysical processes in a bulk heterojunction system using a soluble poly(p-phenylenevinylene) donor and a novel small molecular electron acceptor based on Vinazene (2-vinyl-4,5-dicyanoimidazole). Recent work has shown that this blend exhibits a featureless emission, prominent at long wavelengths of the spectrum, which was attributed to a CT-exciton [J. Chem. Phys. 2009, 130, 094703]. We monitored the field induced dissociation of these CT-excitons by means of steady state and time resolved PL spectroscopy. Shortened decay times and reduced PL emission in blend film evidence the dissociation of the emissive intermolecular pair by the external electric field. Analyzing the dependence of the photocurrent and external quantum efficiency on the external field, the fate of the separated exciplex pairs is tackled. It is suggested that the formation of free carriers involves channels other than CT-excitons in such blends.

DS 17.5 Tue 14:45 H37

Study of Sub-Bandgap States in Polymer-Fullerene Solar Cells — •Martin Presselt[1], Felix Herrmann[1], Marco Seeland[1], Maik Bärenklau[1], Sebastian Engmann[1], Roland Rösch[1], Wichard J. D. Beenken[2], Sviatoslav Shokhovets[1], Harald Hoppe[1], and Gerhard Gobsch[1] — [1]Experimental Physics I, Institute of Physics & Institute of Micro- und Nanotechnologies, Ilmenau University of Technology, Weimarer Str. 32, 98693 Ilmenau, Germany — [2]Theoretical Physics I, Institute of Physics, Ilmenau University of Technology, Weimarer Str. 25, 98693 Ilmenau, Germany

At present polymer-fullerene blends are widely used to build organic solar cells. The main contribution to their photocurrent originates from optical transitions between occupied states below the HOMO level and unoccupied states above the LUMO level of the polymer.

In this work, we investigated the origin of states contributing to the optical absorption in the sub-bandgap spectral range and the resulting photocurrent in P3HT-PCBM bulk heterojunction solar cells. Photothermal deflection spectroscopy, temperature dependent external quantum efficiency, photoluminescence and electroluminescence as well as spectroscopic ellipsometry measurements have been carried out. Effects due to different P3HT-PCBM blending ratios and annealing temperatures have been studied.

Two models are discussed to explain the experimental observations: optical transitions involving (a) disorder and/or defect related states, and (b) charge transfer complexes.

DS 17.6 Tue 15:00 H37

Influence of system size on simulated charge mobility in amorphous films of tris(8-hydroxyquinolinato)aluminium (Alq3) — •Alexander Lukyanov and Denis Andrienko — Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany

We present the results of a modeling study of the charge transport in amorphous films of tris(8-hydroxyquinolinato)aluminium (Alq3). In our multiscale approach we combine molecular dynamics to generate material morphologies, Marcus theory to evaluate charge hopping rates and kinetic Monte Carlo to simulate charge dynamics. Energetic disorder is taken into account by assigning partial charges to the hopping sites, obtained from DFT B3LYP, 6-311g(d) calculations. In contrast to the previous studies Poole-Frenkel behavior of the mobility is reproduced. Our results indicate strong finite-size effects, meaning that the absolute value of the calculated mobility decreases with the increase of the simulation box size. Simple analogy with a classical percolation problem suggests that very large systems are required to obtain a reliable estimate of the charge carrier mobility.

DS 17.7 Tue 15:15 H37

Influence of injection and extraction barriers realized by choice of donor and HTL on organic solar cell performance — •Wolfgang Tress, Ellen Siebert, Karl Leo, and Moritz Riede — TU Dresden, Institut für Angewandte Photophysik

In the p-i-n solar cell architecture, the active materials of a donor/acceptor flat heterojunction are sandwiched between two doped transport layers, which provide a highly conductive contact to the cathode metal and the ITO, respectively. This concept allows for a systematic study of the influence of the HOMO of the donor and the adjacent hole transport layer (HTL) on the open circuit voltage (V_{oc}) and the shape of the IV curve. This approach avoids the main problems emerging by metal-organic interfaces like varying work functions, unpredictable interface dipoles, etc.. Additionally, extraction barriers, which cannot be realized by the choice of metal, can be adjusted in a controlled way by a HOMO of the HTL lying deeper than the HOMO of the donor. Using donor and HTL materials with a HOMO between 5.0 and 5.6 eV in combination with C_{60} as acceptor, we demonstrate a systematic dependence of V_{oc} on the HOMO of the donor, whereas the built in field is goverened by the HOMO of the strongly doped HTL. The fill factor (FF) is mainly influenced by the HOMO offset between donor and HTL. Both types of barriers (extraction and injection) decrease FF resulting in s-shaped curves with different characteristics. The experimental results are interpreted by comparison to simulation data of a drift-diffusion model, treating the HOMO barrier with a field dependent lowering effect.

DS 17.8 Tue 15:30 H37

Hole transport characteristics of pentacene studied with Green functions and real-time propagation — •Sebastian Radke[1], Caroline Gollub[1,2], Stanislav Avdoshenko[1], Rafael Gutiérrez[1], and Gianaurelio Cuniberti[1] — [1]Institute for Materials Science and Max Bergmann Center of Biomaterials, Dresden University of Technology — [2]Max Planck Institute for the Physics of complex Systems, Dresden

For temperatures higher than 150 Kelvin the charge carrier mobility in organic semiconductors depends sensitively upon an interplay of band-like and hopping transport [1]. In this contribution, the hole transport characteristics of an organic semiconducting material are studied with two different theoretical methods and both approaches are compared. As a model system a pentacene structure is selected, which is well-characterized in the context of organic electronics. The first approach is based on a Green function formulation of the Holstein-Peierls model, accounting for local and non-local electron-phonon coupling and it addresses the transport problem in the energy space, so that fluctuations are taken into account only within a static picture. In the second approach, a real-time propagation of the charge carrier wave function is performed and this provides a deeper insight into the different time scales appearing in the problem. The Hamiltonian is formulated in the tight-binding representation, where the parametrization is evaluated for different levels of theory of the MD trajectories and of the electronic structure calculations.

[1] Y. C. Cheng, *et al.*, J. Chem. Phys. **118**, 3764 (2002).

DS 17.9 Tue 15:45 H37

Ab initio based modeling of charge transport in organic semiconductors — •Caroline Gollub[1,2], Stanislav Avdoshenko[1], and Gianaurelio Cuniberti[1] — [1]Institute for Materials Science and Max Bergmann Center of Biomaterials, Dresden University of Technology — [2]Max Planck Institute for the Physics of complex Systems, Dresden

In organic electronics, theory is expected to play an important role for the search of organic semiconducting materials with improved charge carrier mobilities. Current theoretical efforts are devoted to the understanding of the charge transport mechanism and the accurate prediction of the structure-mobility relationship. In this contribution, an approach for the charge migration in organic semicondutors is presented based on a self-consistent propagation of the charge carrier wave function effected by the molecular dynamics of the system, i.e. the electronic and nuclear dynamics are treated on an equal footing. The simulation comprises the evaluation of charge transfer parameters from ab initio calculations, the quantum dynamical calculation of the evolution of the charge carrier wave function and the molecular dynamics of the studied system. The method allows to follow the real-time and real-space transport and can be used to extract charge carrier mobilities in dependence of the chemical functionality, the temperature or the structure assembly. The technique will be demonstrated for hole transport in a 1D stack of coronene molecules.

DS 17.10 Tue 16:00 H37

Energetics of Excited States in the Conjugated Polymer Poly(3-hexylthiophene) — Julien Gorenflot[1], •Daniel Mack[1], Daniel Rauh[4], Stefan Krause[2], Carsten Deibel[1], Achim Schöll[2], Friedrich Reinert[2,3], and Vladimir Dyakonov[1,4] — [1]Experimental Physics VI, University of Würzburg, D-97074 Würzburg — [2]Experimental Physics II, University of Würzburg, D-97074 Würzburg — [3]FZK Karlsruhe, Gemeinschaftslabor für Nanoanalytik, D-76021 Karlsruhe — [4]Bavarian Centre for Applied Energy Research (ZAE Bayern), D-97074 Würzburg

Although prototypes and first commercial polymer-based solar panels already exist, a comprehensive understanding of the fundamental processes and energetics involved in photocurrent generation is still missing and limits further device optimisations. We present a complementary set of experiments on poly(3-hexylthiophene(P3HT), which enables us to draw general conclusions on the energy levels and barriers involved in the processes from light absorption to polaron pair dissociation. From photoemission spectroscopy of occupied and unoccupied states we determine the transport gap to 2.6 eV, which we show to be in agreement with the onset of photoconductivity by spectrally resolved photocurrent measurements. We also find that photogenerated singlet excitons, generated with light at the absorption edge, require 0.7 eV of excess energy to overcome the binding energy. The intermediate charge transfer state, also called polaron pair, is situated only 0.3 eV above the singlet exciton. We discuss our results in view of their impact on charge generation.

DS 18: Invited Holý

Time: Wednesday 9:30–10:15 Location: H2

Invited Talk DS 18.1 Wed 9:30 H2

X-ray Scattering Investigations of Ge Quantum-dot Crystals Depositied on Prepatterened Si Substrates — •Vaclav Holý[1], M. Mixa[1], J Stangl[2], T. Fromherz[2], R. T. Lechner[2], E. Wintersberger[2], G. Bauer[2], Ch. Dais[3], E. Müller[3], and D. Grützmacher[3] — [1]Department of Condensed Matter Physics, Faculty of Mathematics and Physics, Charles University in Prague, Czech Republic — [2]Institute for Semiconductor and Solid State Physics, Johannes Kepler University Linz, Austria — [3]Laboratory for Micro- and Nanotechnology, Paul Scherrer Institut, Villigen, Switzerland

We used high-resolution X-ray diffractometry for the investigation of the structure of three-dimensional crystals of Ge quantum-dots grown by a self-organization process during molecular-beam epitaxy of a periodic Ge/Si superlatice on a (001)Si substrate pre-patterned in two dimensions by extreme UV lithography and ion etching (lateral period below 100 nm). Due to a self-organization process driven by the propagation of internal strains from buried dots towards the growing surface, the dot ordering was almost perfectly replicated in all Ge layers in the multilayer stack, resulting in a three-dimensional tetragonal dot "supercrystal". From the reciprocal-space distribution of diffracted X-ray intensity we determined mean parameters of individual dots (shape, size, local chemical composition) and correlation properties of the dot positions. We modeled the self-organization process by a semi-atomic MonteCarlo model, yielding a correlation function of the dot positions that compares well with experimental data.

DS 19: Synthesis of Nanostructured Films by Self-organization I (Focused Session)

Time: Wednesday 10:30–12:45 Location: H2

Topical Talk DS 19.1 Wed 10:30 H2

Glancing angle deposition: Preparation, properties, and application of micro- and nanostructured thin films — •Bernd Rauschenbach, Christian Patzig, Jens Bauer, and Chinmay Khare — Leibniz Institute of Surface Modification, 04318 Leipzig, Permoserstr. 15

Physical vapor deposition under conditions of obliquely incident flux and limited adatom diffusion results in films with a columnar microstructure. An additional substrate rotation can be used to sculpt the columns into various morphologies. This is the basis for glancing angle deposition (GLAD), which generate sculptured thin films with properties that can be designed and realized in a controllable manner. This overview examines the GLAD process and column growth, the properties observed in GLAD produced films, and the applications of this technology. The initial stages of the thin film growth focusing on concepts important to the GLAD process and the effects of ballistic shadowing and surface diffusion, as well as explaining how column morphology evolves during growth are discussed. Deposition onto prepatterned topographies and methods for controlling the column shape, predicting and modelling the column growth are examined. Because this deposition process provides precise nanoscale control over the structure, characteristics such as the mechanical, magnetic and optical properties of the sculptured films may be engineered for various applications. Depositing onto prepatterned substrates forces the columns to adopt a planar ordering, an important requirement for different applications.

DS 19.2 Wed 11:00 H2

Agglomeration kinetics and pattern formation of Pt thin films on yttria stabilized zirconia single crystals — •Henning Galinski, Thomas Ryll, Lukas Schlagenhauf, Anja Bieberle-Hütter, Jennifer M. Rupp, and Ludwig Gauckler — Nonmetallic Inorganic Materials, ETH Zurich, Zurich, Switzerland

Metals and ceramics have distinct diametric bonding characteristics. Thus, the stability of a metal thin film on a ceramic substrate is conditioned by the interactions between the different bonding types across the interface. In the case of weak adhesion the minimization of free surface energies gives rise to decomposition and agglomeration of thin films. Pt thin films with thicknesses up to 180nm were deposited via magnetron and ion-beam sputtering on yttria stabilized zirconia single crystals and subjected to heat treatments up to 1173K for 2 hours. In the case of ion beam sputtering the single crystal has been pre-cleaned in the ion-beam before deposition. The morphological evolution of Pt thin films has been investigated by means of scanning electron microscopy (SEM) and atomic force microscopy (AFM). Three main observations have been made: i) the pre-cleaning has an impact on the morphological evolution of the film during annealing, hence impurities on the surface can be regarded as additional sources for agglomeration. ii) The morphological evolution as function of time has been analyzed by means of Minkowski measures. For the stage of hole coalescences a deviation from the expected Gaussian behaviour is found. iii) The hole growth is in agreement with Brandon and Bradshaw's theory of surface energy driven diffusion.

DS 19.3 Wed 11:15 H2

Self-organized pattern formation on Si by low-energy ion beam erosion with simultaneous Fe incorporation — •Marina Cornejo, Bashkim Ziberi, Frank Frost, and Bernd Rauschenbach — Leibniz-Institut ür Oberflächenmodifizierung (IOM), Permoserstrasse 15, D-04318 Leipzig, Germany

A simple bottom-up approach for the generation of nanostructures on solid surfaces is the low energy ion beam erosion. Under certain sputtering conditions and despite the random nature of the ion bombardment, well ordered nanostructures, like one-dimensional ripples or regular arrays of dots, can be formed by self-organization processes. In the last years, the focus of our group has been the pattern formation by low-energy ion beam erosion, especially the correlation between the experimental parameters and the resulting topography. In this contribution the role of the substrate contamination is introduced. In particular, the incorporation of Fe and its relation with the experimental parameters and the topography evolution on Si was analyzed. For this study a Kaufman-type broad beam source was used. It is shown that with increasing divergence of the ion beam, the concentration Fe found on the Si surface increases and this strongly affects the pattern formation under near normal ion incidence conditions. The Fe originates from an enhanced sputtering of parts of the vacuum chamber. In addition, it is also demonstrated that the steady state concentration of Fe depends on the ion incidence angle. This can be explained by different angular dependence of the sputter yields of Fe and Si, respectively.

DS 19.4 Wed 11:30 H2

In-situ grazing incidence scattering investigations during magnetron sputtering deposition of FePt/Ag thin films — •Jörg Grenzer, Valentina Cantelli, Nicole M. Jeutter, and Johannes von Borany — Institute of Ion Beam Physics and Materials Research, Forschungszentrum Dresden-Rossendorf e.V., P.O. Box 510119, 01314 Dresden, Germany

We report on an in-situ study on the evolution of granular magnetic $L1_0$-FePt/Ag layers deposited by magnetron sputtering on an amorphous SiO_2 substrate. Using synchrotron radiation we investigated the nanostructure growth during deposition as function of the Ag thickness by the simultaneous detection of the cluster growth and of the formation of the hard ferromagnetic $L1_0$-phase applying grazing incidence small-angle X-ray scattering (GISAXS) and X-ray diffraction, respectively.

FePt/Ag nanoparticle were prepared using a dual magnetron deposition chamber, equipped with two Be windows to allow X-ray penetration, that was mounted on the six-circle goniometer of the Rossendorf beam line (ROBL BM20) at the ESRF (European Synchrotron Radiation Facility). The possibility to tune X-ray beam energy, to reduce air scattering and absorption, together with the high brilliance of the synchrotron source had made it possible to obtain a reliable GISAXS signal and to control the cluster morphology during growth even at the initial stage [1].

[1] V. Cantelli, J. von Borany, N.M. Jeutter, J. Grenzer, Adv. Eng. Mat. 11, 478 (2009).

DS 19.5 Wed 11:45 H2

Factors influencing metal impurity induced ion beam patterning of Si(001) — •Sven Macko[1], Frank Frost[2], Bashkim Ziberi[2], Daniel Förster[1], and Thomas Michely[1] — [1]II. Physikalisches Institut, Universität zu Köln, Germany — [2]Leibniz-Institut für Oberflächenmodifizierung e. V., Leipzig, Germany

On Si(001) ion beam pattern formation at angles $\vartheta < 45°$ with respect to the surface normal takes only place in the presence of metal impurities. Here we report experiments addressing the factors influencing impurity induced pattern formation using well controlled UHV experiments. Ion erosion is performed through fluences $> 5 \times 10^{21}$ ions/m^2 of 2 keV Kr$^+$ with a differentially pumped fine focus ion source. Codeposition of metal impurities is performed through co-sputtering and co-evaporation of Fe. With increasing Fe concentration under otherwise identical conditions a smooth unpatterned surface, a dot pattern and finally for the highest Fe concentrations a ripple pattern is observed. Co-sputtering measurements at temperatures below and above room temperature lead to identical pattern sequences. Thus thermal diffusion is irrelevant for ion beam pattern formation on Si(001) at room temperature. Finally, the orientation of ripple patterns appears to be associated with the direction of impinging Fe atoms.

DS 19.6 Wed 12:00 H2

Dependence of wavelength of Xe ion-induced rippled structures on the fluence in the medium ion energy range — •Antje Hanisch[1], Andreas Biermanns[2], Jörg Grenzer[1], and Ullrich Pietsch[2] — [1]Institute of Ion Beam Physics and Materials Research, Bautzner Landstrasse 400, 01328 Dresden, Germany — [2]Institute of Physics, University of Siegen, Walter Flex 3, 57078 Siegen, Germany

Ion-beam eroded self-organized nanostructures on semiconductors offer new ways for the fabrication of high density memory and optoelectronic devices. It is known that wavelength and amplitude of noble gas ion-induced rippled structures tune with the ion energy and the fluence depending on the energy range, ion type and substrate. The linear theory by Makeev [1] predicts a linear dependence of the ion energy on the wavelength for low temperatures. For Ar$^+$ and O_2^+ it was observed by different groups [2] that the wavelength grows with increasing fluence after being constant up to an onset fluence and before saturation. In this coarsening regime power-law or exponential behavior of the wavelength with the fluence was monitored. So far, investigations for Xe ions on silicon surfaces mainly concentrated on energies below 1keV. We found a linear dependence of both the ion energy and the fluence on the wavelength and amplitude of rippled structures over a wide range of the Xe$^+$ ion energy between 5 and 70keV. Moreover, we estimated the ratio of wavelength to amplitude to be constant meaning a shape stability when a threshold fluence of 2x10^{17}cm^{-2} was exceeded.

[1] Makeev et al., NIM B 197, 185-227 (2002) [2] Karmakar et al., APL, 103102 (2008), Datta et al., PRB 76, 075323 (2007)

Topical Talk DS 19.7 Wed 12:15 H2

Synthesis of Nanostructured Films by Self-organization — •Hans Hofsäss — II. Physikalisches Institut, Universität Göttingen, Göttingen, Germany

Two approaches to achieve self-organized formation of nanostructured thin films will be discussed. In the first approach, nanocomoposite films are prepared by simultaneous deposition of two desired constitutents, e.g. the formation of metal-carbon nanocomposites by simultaneous metal and carbon ion deposition [1]. Depending on the phase diagram one would expect a homogeneous alloy or nanocomposite system. Instead, one often observes multilayered films with alternating metal and carbon layers. The formation of such layered films is explained by self-organization caused by surface segregation, clustering, sputtering and ion induced diffusion. A growth model taking into account these processes allows to predict the transition between self-organized multilayer formation and formation of homogeneous nanocomposites as function of ion energy and ion flux ratio. The second approach is surfactant sputtering [2], i.e. sputter erosion of a substrate, simultaneously exposed to a weak flux of surfactant atoms. Depending on the surfactant-substrate combination self-organized nanostructured ultrathin films are formed as a steady-state. This leads to the generation of novel surface patterns and surface nanostructures. Selected examples of will be discussed. [1] H. Hofsäss and K. Zhang, Appl. Phys. A: Mat. Sci. Proc. 92 (2008) 517 [2] I. Gerhards, H. Stillrich, C. Ronning, H. Hofsäss and M. Seibt, Phys. Rev. B70 (2004) 245418

DS 20: Gaede-Prize Talk (Linden, Stefan)

Time: Wednesday 14:00–14:45 Location: H36

Prize Talk DS 20.1 Wed 14:00 H36

Photonic Metamaterials: Novel Optics with Artificial Atoms — •Stefan Linden — Institut für Nanotechnologie, Karlsruher Institut für Technologie (KIT)

At optical frequencies, electromagnetic waves interact with natural materials via the electronic polarizability of the materials. By contrast, the corresponding magnetizability is negligible. As a result, we can only directly manipulate the electric component of light while we have no immediate handle on the magnetic component. Photonic metamaterials open up a way to overcome this constraint. The basic idea is to create an artificial crystal with sub-wavelength periods. Analogous to an ordinary optical material, such a photonic metamaterial can be treated as an effective medium. However, proper design of the elementary building blocks ("artificial atoms") of the photonic metamaterial allows for a non-vanishing magnetic response at optical frequencies - despite the fact that photonic metamaterial consist of non-magnetic constituents. This artificial magnetism can even lead to a negative index of refraction. In this presentation, I will review our results and present new developments in this interesting field.

DS 21: Invited Babonneau

Time: Wednesday 15:00–15:45 Location: H2

Invited Talk DS 21.1 Wed 15:00 H2

Self-organization of noble-metal nanoparticles on rippled dielectric surfaces produced by low-energy ion erosion — •David Babonneau, Sophie Camelio, and Lionel Simonot — Institut PPRIMME, Poitiers, France

A new route to control the morphology and the spatial organization of metallic nanoparticles, and therefore their physical properties, is to use nanostructured surfaces as templates. We will report on the development of an original approach that integrates the production of nanoripple patterns with long-range order by Xe$^+$ ion-etching of amorphous dielectric films (Al_2O_3, BN, Si_3N_4) and the elaboration of organized arrays of aligned Au and Ag nanoparticles by grazing incidence ion-beam sputtering. By combining direct imaging methods (TEM, AFM) and grazing incidence small-angle X-ray scattering (GISAXS) experiments associated with quantitative analysis, we will show that valuable information can be obtained on the morphology as well as lateral and vertical correlations of the nanostructures present in the nanocomposite films (i.e., ripples, nanoparticles, and surface roughness of the capping layer). In particular, shadowing effects due to the grazing incidence geometry lead to the formation of self-organized nanoparticles with an ellipsoidal shape and a major axis parallel to the ripples. The optical properties of the metallic nanoparticles deposited onto such unidimensional patterns of nanoripples exhibit a strong dependence on the light polarization, which can interpreted as the consequence of both the in-plane spatial organization of the nanoparticles and their shape anisotropy.

DS 22: Synthesis of Nanostructured Films by Self-organization II (Focused Session)

Time: Wednesday 16:00–17:45 Location: H2

Topical Talk DS 22.1 Wed 16:00 H2

Self-organization during the growth of phase-separated nanostructured thin films — •Gintautas Abrasonis — Institute of Ion Beam Physics and Materials Research, Forschungszentrum Dresden-Rossendorf, PF-510119, 01314 Dresden, Germany — School of Physics, University of Sydney, New South Wales 2006, Australia

Control over the morphology and spatial correlations at the nanoscale is one of the major challenge of the nowadays nanoscience and nanotechnology. Bottom-up approaches to nanostructured material synthesis are based on self-organization processes to precisely define ordered nanostructures on a large scale. Self-organization occurs via the interplay between two factors - an external constraint acting on internal system processes. During the thin film growth this is translated into the interplay between thermodynamic driving forces and kinetic constraints. In this talk I will summarize the recent research activities of our group on the phase separation during the growth of carbon-transition metal thin films. Different processes can be 'switched off/on' by external control of the experimental parameters such as temperature, substrate type, matrix/dispersed phase chemical affinity or incoming particle energy. This results in a large variety of lateral or vertical composition modulations, such as encapsulated nanoparticles, high aspect ratio nanocolumns or self-organized layered 3D nanoparticle arrays. Such self-organization process is versatile as different carbon-transition metal systems show this effect. The observed tendencies will be discussed on the basis of the interplay of thermal and energetic ion induced phenomena.

DS 22.2 Wed 16:30 H2

Biaxial optical anisotropy of self aligned silver nanoparticles and nanowires — •Mukesh Ranjan, Stefan Facsko, and Wolfhard Möller — Forschungszentrum Dresden-Rossendorf, Dresden, Germany

In the present study ion beam sputtering has been used for prestructuring of a silicon substrate followed deposition of metal by e-beam evaporation. First a low energy ion beam (Ar^+, 500 eV) is incident on the substrate surface at an angle of 67° to the surface normal to produce well ordered (20-50 nm)ripple patterns. Then physically vaporized Ag atoms are deposited at grazing angle of 70° to the surface normal and normal to the ripples direction. Varying deposition parameters, i.e. ripple periodicity, substrate temperature and atomic flux, we were able to produce well ordered nanoparticles and nanowires. Self-aligned Ag nanoparticles and nanowires deposited on pre-patterned ripple surfaces exhibit strong optical anisotropy. Generalised ellipsometry measurements show that off diagonal Jones matrix elements (Ψ_{ps}, Δ_{ps}, Ψ_{sp}, Δ_{sp}) are non zero and vary with Eulers angle φ. This indicates that such a medium is biaxial in nature. A biaxial layer model approach is used to calculate dielectric functions for such a system. Tauc-Lorentz oscillators are used along x and y direction independently and Drude model along z-direction for nanoparticles. This approach provides a very good fitting with the measured Jones matrix element Ψ_{pp}, Δ_{pp}, Ψ_{ps}, Δ_{ps}, Ψ_{sp}, Δ_{sp}. Different cases for ordered nanoparticles and wires will be presented.

DS 22.3 Wed 16:45 H2

Growth of quantum dot crystals in amorphous matrix on rippled substrates — •Maja Buljan[1,2], Jörg Grenzer[3], Adrian Keller[3], Nikola Radić[2], Thomas Cornelius[4], Till Harmut Metzger[4], and Vaclav Holý[1] — [1]Faculty of Mathematics and Physics, Charles University in Prague, 12116 Prague, Czech Republic — [2]Ruder Bošković Institute, Bijenička c. 54, 10000 Zagreb, Croatia — [3]Forschungszentrum Dresden-Rossendorf, e.V. P.O. Box 10119, 01314 Dresden, Germany — [4]European Synchrotron Radiation Facility (ESRF), BP 220, F-38043, Grenoble, France

The formation of quantum dot crystals by multilayer deposition has been reported and explained satisfactorily only in crystalline materials, so far. Here we demonstrate a method for the growth of quantum dot crystals in amorphous matrices. The ordering of the positions of quantum dots is induced by the deposition of a multilayer on a periodically rippled substrate at an elevated substrate temperature. During the deposition, the quantum dots self-arrange following the morphology of the substrate. The result is a formation of well ordered lattice of Ge quantum dots in amorphous silica matrix. We have investigated the ordering of the dots by grazing-incidence small-angle X-ray scattering and we found that the distance of the dots in the multilayer interfaces close to the rippled surface indeed equals the ripple period. However, in more distant interfaces the dot-dot distance approaches the value for non-rippled substrate and the dot ordering is slightly less pronounced. This finding confirms the beneficial influence of the rippled substrate on the ordering of quantum dots in an amorphous matrix.

DS 22.4 Wed 17:00 H2

Kinetic Monte Carlo simulation of a three-dimensional Si/Ge quantum-dot crystal growth — •Martin Mixa and Václav Holý — Department of Condensed Matter Physics, Charles University, Ke Karlovu 5, 121 16 Prague, Czech Republic

A very regular three-dimensional (3D) arrangement of quantum dots can be achieved by a self-organized growth taking place on a prepatterned substrate. This growth technique has been successfully used at fabrication of 3D quantum-dot crystal of Ge dots in a Si matrix grown on a prepatterned Si(001) surface [1,2].

In our theoretical study we use the kinetic Monte Carlo method for simulation of such a Ge/Si(001) superlattice growth. We developed an efficient and simple kinetic Monte Carlo model [3] describing the surface diffusion and coalescence of deposited adatoms, whereas the shape of the growing dots is not atomistically simulated (it is taken ad hoc from the experiment). The self-organization effect is incorporated in the model via an influence of the strain field induced by buried dots on the hopping probabilities of migrating adatoms.

[1] D. Grützmacher et al., Nano Lett. 7, 3150 (2007). [2] V. Holý et al., Phys. Rev. B 79, 035324 (2009). [3] M. Mixa et al., Phys. Rev. B 80, 045325 (2009).

Topical Talk DS 22.5 Wed 17:15 H2

Self-organization and molecular diffusion processes in organic thin film growth — •Christian Teichert — Institute of Physics, University of Leoben, A-8700 Leoben, Austria

Crystalline films of conjugated organic semiconductors offer attractive potential for optoelectronic and electronic applications on flexible substrates. Due to the complexity and anisotropy of the molecular building blocks, novel growth mechanisms can occur as is demonstrated for the growth of the rod-like oligophenylene molecule parasexiphenyl (6P) on mica surfaces. On clean mica(001), the self-organization of crystallites into one-dimensional chains is observed on a wetting layer where the 6P molecules lie on the surface [1]. However, if the mica surface is amorphized by gentle bombardment with 500 eV Ar^+ ions, the formation of terraced mounds composed by almost upright standing molecules is found by atomic force microscopy. Quantitative analysis of the morphology together with transition state theory calculations revealed the existence of level dependent step edge barriers [2]. A lower barrier due to less molecular tilt in the first layer results in the completion of one monolayer before mound formation starts.

[1] C. Teichert, et al., Appl. Phys. A 82 (2006) 665. [2] G. Hlawacek, P. Puschnig, P. Frank, A. Winkler, C. Ambrosch-Draxl, C. Teichert, Science 321 (2008) 108.

This work has been performed in collaboration with G. Hlawacek, Q. Shen, S. Lorbek, P. Puschnig, C. Ambrosch-Draxl, P. Frank, and A. Winkler. Support by the Austrian Science Fund (FWF) is acknowledged.

DS 23: High-k and Low-k Dielectrics I (Joint Session DS/DF)

Time: Wednesday 9:30–11:00 Location: H8

DS 23.1 Wed 9:30 H8

Spectroscopic investigations of interaction between C_{60} fullerene and nitrogen atom from amine group — •Jolanta Klocek[1], Daniel Friedrich[1], Kostyantyn Zagorodniy[2], and Dieter Schmeisser[1] — [1]Brandenburgische Technische Universität, LS Angewandte Physik-Sensorik, Konrad-Wachsmann-Allee, 17, 03046, Cottbus, Germany — [2]Institute for Solid State and Materials Research, IFW Dresden, PF 270116, D-01171 Dresden, Germany

We investigated interactions between fullerene molecule and amine group from 3-aminopropyl-trimethoxysilane (3AT). Theoretical calculations show that the material obtained as a result of interactions between 3AT and C_{60} fullerene may have extremely low dielectric constant around 1.6, so it could be considered as a candidate for ultra low-k (ULK) material applications. We prepared films composed of 3AT and fullerene by using two preparation techniques: spin-coating and evaporation. Interactions between these two components were investigated by using X- ray photoelectron spectroscopy (XPS) and Near Edge X-ray Absorption Fine Structure Spectroscopy (NEXAFS). We found that there are strong chemical reactions between the nucleophilic nitrogen atom from 3AT and electrophilic fullerene molecule. Results of NEXAFS measurements suggest that due to direct interactions between 3AT and C_{60} the shape of fullerene molecule is changed.

DS 23.2 Wed 9:45 H8

The influence of elastic and inelastic processes on trap assisted tunnelling through thin dielectric films — •Grzegorz Kozlowski, Jarek Dabrowski, Piotr Dudek, Gunther Lippert, and Grzegorz Lupina — IHP, Im Technologiepark 25, 15236 Frankfurt (Oder) , Germany

Impurities or structural imperfections of the crystal may introduce discrete electronic states (or a band when defects interact with one another) into the band gap of the dielectric. Electrically active defects can be used in a trap assisted tunnelling (TAT) process giving a noticeable contribution to the leakage and to the total current.

We developed a simple quantum mechanical model to investigate the role of defects in leakage current through thin dielectric films for future DRAM applications. The influence of image force as well as a possible charge state of an empty trap was considered. The results of numerical simulation were used to characterize the electrical behaviour of thin dielectric films at different temperatures. The temperature dependence may come from two phenomena. The first one is the Boltzmann distribution of charge carriers in the electrodes. In a limited way one can reproduce the temperature dependence of the leakage by considering various distribution of defects in energy and position in the film. This approach is however insufficient to reproduce the dependence in the whole regime of applied voltages. We thus expanded our model by including an additional type of process, i.e. the electron-phonon coupling which gave rise to non-radiative multiphonon processes.

DS 23.3 Wed 10:00 H8

Electrically optimized high-κ metal gate MOSFET by specific modification of the band alignment — •Łukasz Starzyk, Massimo Tallarida, and Dieter Schmeisser — Brandenburgische Technische Universität, Angewandte Physik-Sensorik, Konrad-Wachsmann-Allee 17, Cottbus D-03046, Germany

The electrical optimization of metal/oxide/semiconductor gate stacks by specific modification of the band alignment for advanced MOS technology incorporating high dielectric constant (κ) materials is explored. Because of requirements concerning continued scaling of MOSFET transistors, gate oxides and cobalt electrode have been grown successively on Si substrate respectively by means of atomic layer deposition (ALD) and evaporation. The thicknesses of high-κ films were around 2 nm. In case of work function engineering, interfaces' chemistry plays a fundamental role. We applied synchrotron radiation based x-ray photoelectron spectroscopy (SR XPS) to characterize our samples, which allows step by step *in situ* investigations. Co 2p, Al 2p, Hf 4f, Si 2p and O 1s core levels spectra were measured and analyzed. From valence band (VB) spectra we determined Schottky barrier height and electronic bands offsets.

DS 23.4 Wed 10:15 H8

A comparison of $(SrO)_x(ZrO_2)_{(1-x)}$ and ZrO_2 as potential high-k dielectric for future memory applications — •Matthias Grube[1], Dominik Martin[1], Walter Michael Weber[1], Thomas Mikolajick[1], Lutz Geelhaar[2], and Henning Riechert[2] — [1]Namlab GmbH, 01187 Dresden — [2]Paul-Drude-Institut für Festkörperelektronik, 10117 Berlin

Following the demands of the aggressive downscaling of the capacitor area of dynamic random access memories, a material screening of novel high-k dielectrics with nanometer-scale thicknesses is required. Pure ZrO_2 and admixtures with SrO are promising examples as possible substitutes for the established materials. Their growth, their physical and electrical characterization is our contribution to the screening. We employed molecular beam deposition to grow thin layers of $(SrO)_x(ZrO_2)_{(1-x)}$ on n^{++}-Si substrates with a predeposited 5nm thin TiN layer as bottom electrode to realize metal-insulator-metal structures. An extensive physical characterisation consisting of X-ray diffraction, X-ray fluorescence analysis, X-ray reflectometry and atomic force microscopy was performed to verify the crystallinity, the stoichiometry, the physical thickness and the surface morphology of the dielectric film itself. The interface between the dielectric and the bottom electrode was investigated by transition electron microscopy. I-V and C-V measurements revealed k-values consistent to the literature for ZrO_2. However, for $(SrO)_x(ZrO_2)_{(1-x)}$ rather low k-values below 9 for films up to 20 nm and much higher k-values of about 50 for films of 40 nm thickness were observed. Those dependencies will be discussed.

DS 23.5 Wed 10:30 H8

Nanoscale analysis of the electric properties of ultra thin ZrO_2-, $(ZrO_2)_x(Al_2O_3)_{1-x}$- and $ZrO_2/Al_2O_3/ZrO_2$-films. — •Dominik Martin[1], Matthias Grube[1], Elke Erben[1], Wenke Weinreich[2], Uwe Schröder[1], Lutz Geelhaar[3], Walter Weber[1], Henning Riechert[3], and Thomas Mikolajick[1] — [1]namlab Gmbh, D-01187 Dresden — [2]Fraunhofer-CNT, D-01099 Dresden — [3]Paul-Drude-Institut für Festkörperelektronik, D-10117 Berlin

In order to achieve an high k-value in sub 10 nm thin films of ZrO_2 it is necessary to reach the tetragonal crystalline phase. This is done by either depositing the layer at higher temperatures or by a post deposition annealing step. Both however induce high leakage current through the layer. Small amounts of Al_2O_3 can be incorporated in ZrO_2 to reduce leakage current. In order to understand the detailed charge carrier transport mechanisms, thickness series of ultra thin ZrO_2-, $(ZrO_2)_x(Al_2O_3)_{1-x}$- and $ZrO_2/Al_2O_3/ZrO_2$-films were deposited by Atomic Layer Deposition and subjected to different rapid thermal annealing processes. These layers were examined by I-V-, C-V-Spectroscopy and conductive atomic force microscopy. It is shown that Al incorporation throughout the entire layer imposes the relatively low k value of Al_2O_3 onto the entire layer. Whereas incorporation of only to cycles of Al into the center of the ZrO_2 effectively reduces leakage currents while maintaining a higher k value.

DS 23.6 Wed 10:45 H8

Atomic Vapour Deposition of TiTaO for MIM applications — •Mindaugas Lukosius[1], Canan Baristiran Kaynak[1], Christian Wenger[1], Günther Ruhl[2], and Simon Rushworth[3] — [1]IHP, Technologiepark 25, 15236 Frankfurt Oder, Germany — [2]Infineon, Wernerwerkstr. 2, 93049 Regensburg, Germany — [3]SAFC HiTech, Bromborough, Wirral, Merseyside, U.K. CH62 3QF

Metal-Insulator-Metal (MIM) capacitors are widely used in ICs for Radio-Frequency (RF) applications. Currently, capacitors fabricated by performing MIM structures use silicon oxide or silicon nitride as an insulating layer. However, the capacitance density of these materials is limited by low dielectric constant values. Therefore, for further integration of passive components such as capacitors into CMOS devices, dielectric materials with higher permittivity than SiO2 (k = 3.8) are required. Atomic Vapor Deposition (AVD*) technique was successfully applied for the first time for depositions of TiTaO oxide films on 8-inch wafers using two separate Ti(OPri)2(mmp)2 and TBTDET precursors for MIM applications in back-end of line (BEOL). Composition, crystalinity and electrical properties such as dielectric constant, capacitance and leakage currents were studied in Au/TiTaO/TiN/Si MIM capacitors. The effect of post deposition annealing (PDA) and investigation of different top electrode materials will be also presented.

DS 24: High-k and Low-k Dielectrics II (Joint Session DS/DF)

Time: Wednesday 11:15–12:45 Location: H8

DS 24.1 Wed 11:15 H8

Electrical and structural characteristics of SrTaO/SrTiO based M-I-M capacitors — •Canan Baristiran Kaynak[1], Mindaugas Lukosius[1], Bernd Tillack[1], Christian Wenger[1], Guenther Ruhl[2], and Tom Blomberg[3] — [1]IHP Im Technologiepark 25, 15236 Frankfurt Oder, Germany — [2]Infineon Technologies AG, Wernerwerkstr. 2, 93049 Regensburg, Germany — [3]ASM Microchemistry Ltd., Väinö Auerin katu 12 A, 00560 Helsinki, Finland

In this work, on-chip M-I-M capacitors are realized using SrTiO /SrTaO dielectric stacks. The deposition of the SrTiO dielectric is done by ALD and to get a crystalline state correspondingly high k value, 550 °C annealing temperature is applied. Moreover, SrTaO is considered as a part of barrier stack due to its amorphous characteristic at 550°C annealing temperatures. In this way, it is expected to improve the electrical characteristic of the devices. A set of M-I-M stacks such as Au/SrTiO/TaN/Si, Au/SrTaO/SrTiO/TaN/Si and Au/SrTiO/SrTaO/TaN/Si have been deposited and analyzed by means of electrical and analytical characterizations. The effect of thickness of SrTaO was also evaluated. From the C-V and J-V measurements, dielectric constant, corresponding capacitance densities and leakage current performance were extracted. For the investigation of interfaces between the stacks XPS and ToF-SIMS were utilized. The results mainly demonstrate that the use of SrTaO material in the barrier stack strongly improves the leakage current density of M-I-M capacitors due to its amorphous state which serves as a strong barrier between the dielectric and the electrode of the M-I-M capacitor.

DS 24.2 Wed 11:30 H8

Resistive switching in TiN/HfO_2/Ti/TiN MIM structures for future memory applications — •Christian Walczyk[1], Christian Wenger[1], Mindaugas Lukosius[1], Mirko Fraschke[1], Ioan Costina[1], Sebastian Schulze[1], Sebastian Thiess[2], Wolfgang Drube[2], and Thomas Schroeder[1] — [1]IHP, Im Technologiepark 25, 15236 Frankfurt (Oder), Germany. — [2]Hasylab at DESY, Notkestrasse 85, 22607 Hamburg, Germany.

The electrically switchable resistance change phenomenon between a high (OFF-state) and a low (ON-state) resistive state of a metal-insulator-metal (MIM) diode structure has attracted considerable attention in recent years for future non-volatile memory applications (RRAM). Especially hafnium dioxide (HfO_2) as insulator is among the oxides particularly desirable due to the fact that it is nowadays considered as a BEOL Si CMOS compatible binary metal oxide system. Typical bipolar current-voltage characteristics of a TiN/HfO_2/Ti/TiN stack with a HfO_2 thickness of 10 nm will be presented. The switching properties crucially depend on a) whether the additional Ti layer is integrated as top or bottom electrode and b) on the application of post-deposition annealings (PDA). To unveil the origin of these observations, a materials science study by TOF-SIMS, TEM and HAXPS was carried out. It is possible to prove that this metallic Ti layer getters during the PDA treatments oxygen from HfO_2, resulting in the formation of non-stoichiometric HfO_x. Due to their significance in NVM technology, we will furthermore present the retention and cycling endurance characteristics.

DS 24.3 Wed 11:45 H8

Oxygen Engineering of HfO_{2-x} Thin Films grown by Reactive Molecular Beam Epitaxy — •Erwin Hildebrandt[1], Jose Kurian[1], Peter Zaumseil[2], Thomas Schröder[2], and Lambert Alff[1] — [1]Institut für Materialwissenschaft, TU-Darmstadt — [2]IHP, Frankfurt, Oder

Reactive Molecular Beam Epitaxy (R-MBE) is an ideal tool for tailoring physical properties of thin films to specific needs. For the development of cutting-edge oxides for thin film applications a precise control of oxygen defects is crucial. R-MBE in combination with rf-activated oxygen allows reproducibly growing oxide thin films with precise oxidation conditions enabling oxygen engineering.

R-MBE was used to grow Hf and $HfO_{2\pm x}$ thin films with different oxidation conditions on sapphire single crystal substrates. Structural characterization was carried out using rotating anode x-ray diffraction revealing highly textured to epitaxial thin films on *c*-cut sapphire. Furthermore, switching of film orientation by varying the oxidation conditions was observed demonstrating the role of oxygen in the growth procedure. The investigation of electrical properties using a four probe measurement setup showed conductivities in the range of 1000 $\mu\Omega$cm for oxygen deficient HfO_{2-x} thin films. Optical properties were investigated using a photospectrometer and additionally x-ray photoelectron spectroscopy was carried out to study the band gap and valence states. Both techniques were used to monitor the oxygen content in deficient HfO_{2-x} thin films. Our results demonstrate the importance of oxygen engineering even in the case of 'simple' oxides.

DS 24.4 Wed 12:00 H8

Band structure and electrical properties of MBE grown HfO_2 - based alkaline earth perovskites — •Dudek Peter[1], Łupina Grzegorz[1], Kozłowski Grzegorz[1], Dabrowski Jarek[1], Lippert Gunther[1], Müssig Hans-Joachim[1], Schmeisser Dieter[2], and Schroeder Thomas[1] — [1]IHP-Microelectronics, Im Technologiepark 25, D-15236 Frankfurt (Oder) — [2]BTU Cottbus, Konrad-Wachsmann-Allee 17, D-03046 Cottbus, Germany

Ultra thin dielectric films (<20 nm) deposited on TiN electrodes are interesting for MIM capacitor application. High capacitance density and dielectric permittivity must be accompanied by extremely low leakage currents (10^{-8} A/cm^2) at bias 0.5 V. To achieve such low leakage currents, high band gap and proper band alignment is required. Occupied electronic states can be probed with standard laboratory photoemission methods. Probing of unoccupied states is more challenging. Synchrotron based PES in combination with XAS forms a powerful method to study the band alignment. ASAM end station located at the U 49/2 PGM 2 beamline of BESSY II (Berlin) offers excellent conditions for performing such measurements. We investigated HfO_2 - based alkaline earth perovskite - $BaHfO_3$ with subsequent admixture of TiO_2, resulting in formation of $BaHf_{0.5}Ti_{0.5}O_3$ compound. The analysis of data indicates that band gap for HfO_2 is similar to $BaHfO_3$ and amounts 5.8 eV; for $BaHf_{0.5}Ti_{0.5}O_3$ it decreases to 3.8 eV. We conclude that the addition of TiO_2 to $BaHfO_3$ increases significantly the dielectric permittivity but also impacts the band gap alignment. The conduction band offset shrinks, influencing the leakage current behavior.

DS 24.5 Wed 12:15 H8

In-situ EELS and UPS measurements on HfO_2 ALD layers — •Marcel Michling, Massimo Tallarida, Krzysztof Kolanek, and Dieter Schmeisser — Brandenburgische Technische Universität Cottbus, Angewandte Physik/Sensorik, K.-Wachsmann-Allee 1, 03046 Cottbus

In this contribution we report on our in-situ cycle-by-cycle (up to 10 cycles) investigations of the HfO_2 ALD process using the methods of EELS and UPS.

We used TDMA-Hf as a precursor and p-type Si wafer with natural oxide as the substrate. The EELS measurements were done with a primary energy of 52,5 eV and the UPS measurements with He I (21,218 eV).

The change in the onset of the loss function is readily observed. Already after two cycles the value approach to the bulk value of HfO_2. Upon ALD growth there is a remarkable decrease in the intensity of states within the gap. They are rather smooth and saturate after 10 cycles. With UPS we follow the variation of the VB onset and changes in the secondary electron onset. We summarize our data in a band diagram not based on bulk values but on cycle dependent quantities. With these cycle-by-cycle experiments we study the initial growth of HfO_2 especially in the very first cycles.

DS 24.6 Wed 12:30 H8

Determination of interfacial layers in high - k ALD nanolaminate materials by ARXPS and SRXPS measurements. — •Jakub Wyrodek[1], Massimo Tallarida[1], Dieter Schmeisser[1], and Martin Weisheit[2] — [1]Brandenburgische Technische Universität, Angewandte Physik-Sensorik, Konrad-Wachsmann-Allee 17, Cottbus D-03046, Germany — [2]GLOBALFOUNDRIES, Dresden, Germany

The interfacial layers of high dielectric constant (high - k) nanolaminate films are here explored. Problems concerning ALD nanolaminate layers deals mainly with lack of accurate methods to determine in depth profile of few nm thick stacks. Modified angle resolved XPS(ARXPS) and synchrotron radiation XPS(SRXPS) are proposed as methods suitable in layer profiling. Studied stacks containing ZrO/HfO or AlO/ZrO, were prepared on Si substrates by atomic layer deposition (ALD). Two sets of experiments were covered. First dealt with initial growth (up to 20 cycles, with thickness d $<$ 2nm) of AlO/ZrO and included layer by layer *insitu* investigation by SRXPS. Second experiment refer to industrial grown ZrO/HfO films (d $\sim$ 3nm) processed with various parameters resulting in both, layer by layer and homogenous depositions. For those samples *exsitu* XPS, with angle dependent variation of probing depth, measurements were covered. By comparing obtained intensity ratios for different angles with computational developed stack model it was found that no simple layer by layer but some intermixing growth occurred including interaction with silicon substrate.

DS 25: Application of Thin Films

Time: Wednesday 16:00–17:00 Location: H8

DS 25.1 Wed 16:00 H8

Development of Multilayer Laue Lenses for soft X-ray radiation — •Tobias Liese[1], Hans-Ulrich Krebs[1], Michael Reese[2], Peter Grossmann[2], and Klaus Mann[2] — [1]Institut für Materialphysik, Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen — [2]Laser-Laboratorium Göttingen e.V., Hans-Adolf-Krebs-Weg 1, 37077 Göttingen

Despite the improvements of fabrication techniques for Fresnel Zone Plates as diffractive optics for X-ray microscopy, the spatial resolution with high diffraction efficiencies has reached a limit mostly. A novel approach to focusing soft X-rays in the water window regime (2.3 – 4.4 nm) is to prepare non-periodic multilayer structures using as 1-dimensional zone plates in Laue diffraction geometry. For this purpose ZrO_2/Ti multilayers were deposited by pulsed laser deposition (PLD) on Si(111) substrates in ultrahigh vacuum. The interfaces within the multilayer are positioned according to the Fresnel zone plate law. In this contribution, results of the Laue Lens fabrication by focused ion beam (FIB) and lens characteristics measured by a table-top X-ray source are presented.

DS 25.2 Wed 16:15 H8

AlN-basierte Mikrogeneratoren — •Oliver Bludau, Claus-Christian Röhlig, Lutz Kirste, Ram Ekwal Sah, Rachid Driad, Vadim Lebedev, Volker Cimalla, Christoph Nebel und Oliver Ambacher — Fraunhofer Institut für Angewandte Festkörperphysik IAF, Freiburg

Auf Basis mikromechanischer Resonatorstrukturen (Cantilever) wurden Mikrogeneratoren entwickelt, mit denen im menschlichen Körper vorhandene mechanische Energie (Vibrationen) in elektrische Energie umgesetzt werden kann. Diese Mikrogeneratoren sollen in der Lage sein, implantierte Sensorsysteme mit Energie zu versorgen. Für die Energiewandlung wurden piezoaktive (c-Achsen orientierte) Aluminiumnitrid (AlN)-Dünnschichten (d = 200 nm) in einem RF-Magnetron Sputterprozess abgeschieden und mittels Röntgen-Diffraktometrie charakterisiert. Der piezoelektrische Modul (d_{33}) der Schichten wurde mit Piezoelektrischer Kraftmikroskopie und Laser-Doppler Vibrometrie gemessen. Die Cantilever wurden extern angeregt und die durch die Dehnung der AlN-Schicht generierte Piezospannung mit einem Oszilloskop gemessen. Zudem erfolgte eine Untersuchung der Resonanzfrequenzen und der Gütefaktoren der Strukturen. Aufgrund der hohen piezoelektrischen Konstanten (e_{33} = 1,5 C/m^2), der chemischen Stabilität in wässrigen Lösungen sowie der vorhandenen Biokompatibilität, ist eine Wandlung der im menschlichen Körper vorhandenen mechanischen Energie in elektrische Energie zum Betrieb implantierter Sensoren mit einigen Mikrowatt möglich.

DS 25.3 Wed 16:30 H8

Aluminum Nitride and Nanodiamond Thin Film Microstructures — •Fabian Knöbber, Oliver Bludau, Claus-Christian Röhlig, Oliver Williams, Ram Ekwal Sah, Lutz Kirste, Volker Cimalla, Vadim Lebedev, Christoph Nebel, and Oliver Ambacher — Fraunhofer-Institute for Applied Solid State Physics, Freiburg, Germany

In this work, aluminum nitride (AlN) and nanocrystalline diamond (NCD) thin film microstructures have been developed. Freestanding NCD membranes were coated with a piezoelectrical AlN layer in order to build tunable micro-lens arrays. For the evaluation of the single material quality, AlN and NCD thin films on silicon substrates were fabricated using RF magnetron sputtering and microwave chemical vapor deposition techniques, respectively. The crystal quality of AlN was investigated by X-ray diffraction. The piezoelectric constant d_{33} was determined by scanning laser vibrometry. The NCD thin films were optimized with respect to surface roughness, mechanical stability, intrinsic stress and transparency. To determine the mechanical properties of the materials, both, micromechanical resonator and membrane structures were fabricated and measured by magnetomotive resonant frequency spectroscopy and bulging experiments, respectively. Finally, the behavior of AlN/NCD heterostructures was modeled using the finite element method and the first structures were characterized by piezoelectrical measurements.

DS 25.4 Wed 16:45 H8

Single Ion Lithography — •Hans-Gregor Gehrke[1], Anne-Katrin Nix[1], Johann Krauser[2], Christina Trautmann[3], Alois Weidinger[4], and Hans Hofsäss[1] — [1]II. Physikalisches Institut, Universität Göttingen, Germany — [2]Hochschule Harz, Wernigerode, Germany — [3]Gesellschaft für Schwerionenforschung, Darmstadt, Germany — [4]Hahn-Meitner-Institut, Berlin, Germany

Swift Heavy ion irradiation of polycarbonate creates latent tracks along each ion track. Chemical wet etching allows selective removal of the path creating small pores through the polymer film. In the past we developed a method to create thin polycarbonate films by spin coating allowing the etching of pores with diameters in the range of 50 - 80 nm. These nano-pores serve as templates to create nanostructures. Besides depositing materials through the pores, it is possible to sputter cavities into the substrate. This technique has some possible applications, as for example, the creation of structured substrates for nano-wires requiring small catalyst clusters (e.g. gold). The combination of creating cavities by sputtering and depositing the catalyst into cavities results in embedded catalyst clusters providing advantages for epitaxial growth. In addition, this procedure is a parallel process allowing to structure large areas with millions of devices simultaneously. Another application is the creation of electrode structures. We demonstrate the principle of creating a field emission structure using the described structuring method and the self-alignment of conducting nano-wires in diamond-like carbon created by the same ion during irradiation.

DS 26: [CPP] Organic Electronics and Photovoltaics III (Joint Session DS/CPP/HL/O)

Time: Wednesday 9:30–12:45 Location: H37

DS 26.1 Wed 9:30 H37

High-resolution spectroscopic mapping of P3HT:PCBM organic blend films for solar-cell applications — •Xiao Wang[1], Dai Zhang[1], Kai Braun[1], Hans-Joachim Egelhaaf[2], Christoph J. Brabec[2], and Alfred J. Meixner[1] — [1]Institute of Physical and Theoretical Chemistry, University of Tübingen — [2]Konarka Technologies GmbH, Nürnberg

We present a high resolution near-field spectroscopic mapping of the poly(3-hexylthiophene) and [6, 6]-penyl-C61 butyric acid methyl ester (P3HT:PCBM) blend film upon different thermal annealing.[1] From the simultaneously recorded morphology and spectroscopic information, the interplay among the blend film morphology, the local P3HT:PCBM molecular distribution, and the P3HT photoluminescence (PL) quenching efficiency were discussed. The PL and Raman signals of the electron donor (P3HT) and acceptor (PCBM) have been probed at an optical resolution of approximately 10 nm which allow the direct identification of the chemical nature of the different domains. Moreover, we were able to reveal and quantify local quenching, which is related to the electron transfer from P3HT to PCBM. Based on the experimental results, it is proposed that high resolution near-field spectroscopic imaging proves its clear capability of mapping the local chemical composition and photophysics of the P3HT:PCBM blends on a length of a few nanometers.

[1] X. Wang, et al. Advanced Functional Materials (in press)

DS 26.2 Wed 9:45 H37

Investigations on thickness dependence of electrical characteristics and stability of self-assembled monolayers — •Dana Habich — FAU Erlangen-Nürnberg, Institute of Polymer Materials

We investigated the influence of the molecular chain length (n) of aliphatic Cn-phosphonic acids on the electrical characteristics of self-assembled monolayers (SAMs) based on these molecules. SAMs prepared on aluminium/aluminium oxide (Al/AlOx) and conductive indium tin oxide (ITO) substrates behave as molecular dielectric layer. In integrated devices (e.g. capacitors) with activated Al-bottom electrode, the dielectric layer is created from a double-layer AlOx/SAM. Capacitance and breakdown voltage correlates monotonically with the SAM thickness, the current density at low voltage does not follow the expected correlations in detail. We address this behavior to morphological changes of the SAMs on AlOx, from an amorphous structure for short chains to a crystalline state for longer alkyl chains. To decouple the relative contributions of the AlOx and the SAM to the insulation, an independent analytical approach to characterize the SAM was chosen: cyclic voltammetry on SAM decorated ITO. The faradic current of a redox active compound in solution is indirect proportional to the molecular chain length. Qualitatively, this observation proofs the conclusions from the capacitor measurements. The system ITO/SAM, further provide an approach for functional coatings on ITO with the possibility to tune addressability and stability of the electrodes. Stability was investigated by static contact angle and STM measurements before and after electrical stress. Ref.: Org. Electron. 10 (2009) 1442.

DS 26.3 Wed 10:00 H37

2D mapping of the Electron Beam Induced Current (EBIC) in organic solar cells — •Piet Reuter[1], Thomas Rath[2], Gregor Trimmel[2], and Peter Hadley[1] — [1]Institute of Solid State Physics, TU Graz, A-8010 Graz, Austria — [2]Institute for Chemistry and Technology of Materials & Christian Doppler Laboratory for Nanocomposite Solar Cells, TU Graz, A-8010 Graz, Austria

Electron Beam Induced Current (EBIC) measurements were used to produce 2D nanoscale maps for investigating the homogeneity of solar cells. These maps are acquired by putting the electron beam of a scanning electron microscope (SEM) in spot mode and using a programmable sample stage to move the solar cell under the stationary beam. The electron beam generates electron-hole pairs in the solar cell much like light does in normal operation. The variations in the EBIC signal can be attributed to changes in the morphology. By comparing these measurements with morphological information of the devices, one can identify the cause of inferior performance which should then lead to an improvement of further devices. It should be mentioned that long time exposures to an electron beam destroys the organic semiconductors. Studies were performed to determine the acceptable electron dose during the measurement.

DS 26.4 Wed 10:15 H37

Analysis of Metallic Conduction at the Interface of TTF and TCNQ Crystals. — •Viktor Atalla, Mina Yoon, and Matthias Scheffler — Fritz-Haber-Institut der MPG, Berlin, Germany

Organic materials are promising candidates for a next generation of electronic devices, since they offer a variety of new intriguing electronic phenomena while being environmentally friendly, low cost, and mechanically flexible. Here we study the interface of tetrathiofulvalene (TTF) and 7,7,8,8-tetracyanoquinodimethane (TCNQ) organic molecular crystals which was found to exhibit metallic conduction [1] whereas the individual crystals are large band-gap semiconductors. Using quantum mechanical first-principles approaches employing the FHI-aims code [2] basic properties of monomers, dimers, and individual crystals are investigated. We construct interfaces between the two types of crystals and study the electronic band structures of the interface-induced states, which are relevant to the charge transport properties of the material. Depending on the relative orientation of the crystals the band structures were found to indicate metallic conduction at the interface. Furthermore the energetics of the polaron is investigated by calculating the geometry relaxation energy. For monomers of TTF and TCNQ this is found to be in the order of 0.1 eV, indicating that the electron-lattice interaction is an important parameter for charge transport in this system. [1] H. Alves et al., Nat. Mat. 7, 574 (2008). [2] V. Blum et al., Comp. Phys. Comm. 180, 2175 (2009).

DS 26.5 Wed 10:30 H37

Structural analysis of photoactive polymer blend films on textured polymeric and inorganic substrates — •Robert Meier[1], Matthias A. Ruderer[1], Gunar Kaune[1], Alexander Diethert[1], Fabian Markl[1], Volker Körstgens[1], Johannes Wiedersich[1], Stephan V. Roth[2], and Peter Müller-Buschbaum[1] — [1]TU München, Physik Department LS E13, James-Franck-Straße 1, 85747 Garching — [2]HASYLAB at DESY, Notkestraße 85, 22603 Hamburg

Due to their large chemical variety photoactive conducting polymers are of great interest for versatile applications such as organic photovoltaics. In order to improve the device characteristics not only the polymer film but also the rest of the device has to be optimized regarding light absorption and charge carrier separation. Therefore the focus of this work is put on the use of structured substrates in order to improve the light absorption and the overall device performance. A new route based on solution casting is introduced to structure the electron blocking PEDOT:PSS layer. Absorption spectra of polymer blend films spincoated on such structured substrates show promising aspects for their suitability for organic photovolatics. In addition the inner film morphology of a polymer blend based on M3EH-PPV and F8BT spincoated on structured channel-like substrates is investigated using GISAXS measurements. The obtained results show a dependence of the film morphology and the topographic shape on the etched depth of the channels. The study is complemented with atomic force and scanning electron microscopy measurements.

15 min. break

DS 26.6 Wed 11:00 H37

Structural and morphological changes in P3HT thin film transistors applying an electric field — •Deepak kumar Tiwari[1], Souren Grigorian[1], Ullrich Pietsch[1], Heinz Flesch[1,2], and Roland Resel[1,2] — [1]University of siegen, siegen, Germany — [2]Graz University of technology

We report on electric field dependent crystalline structure and morphological changes of drop casting and spin coated poly(3-hexyltheiopine) (P3HT) thin films. In order to probe the morphological changes induced by an applied electric field the samples were covered with thin source/drain electrodes separated by a small channel of 2 mm width. A series of x-ray reflectivity, X-ray grazing incidence out-of-plane and in-plane scans have been performed as function of the applied electric voltage. The (100) peak shows a decrease in intensity with increase of the applied electric field. This might be caused by Joule heating and the creation of current induced defects in the P3HT film. On other hand the (020) peak intensity shows much stronger changes with applied field. Considering the *-* stacking direction the measured effect can be directly related to a change in the electric transport. The observed changes in structure are reversible and the current-voltage cycle can be repeated several times. For X-ray reflectivity major changes have been found close to critical angle of total external reflection indicating the film becomes less dense and increases in surface roughness with increase of the voltage. This change in surface behaviour could be confirmed by in-situ AFM measurements.

DS 26.7 Wed 11:15 H37

Thickness dependent structural order in P3HT films - a key parameter for high OFET mobility — •Benedikt Gburek, Richa Sharma, Torsten Balster, and Veit Wagner — School of Engineering and Science, Jacobs University Bremen, Campus Ring 1, 28759 Bremen, Germany

Applications of organic electronics require cheap and fast production methods on flexible substrates. Following these goals, top-gate OFETs on PET foils were used to analyze the dependence of the device characteristics on the crucial parameter of semiconductor layer thickness. The organic semiconductor, regio-regular P3HT, and the gate insulator were deposited by spin-coating under atmospheric conditions.

The charge carrier mobility was found to be rather low for extremely thin layers of several nanometers only. However, with increasing layer thickness, mobility increases by two orders of magnitude until a "saturation thickness" of 50 nm, above which it remains constant.

Further details of the ordering were extracted according to the Vissenberg-Matters model with gate-voltage dependent mobility $\mu = \mu_0 \left((V_{GS} - V_{th}) / 1V \right)^{\gamma}$, where γ is directly related to the width of the density of states. The analysis reveals that the disorder parameter γ decreases from 3.1 to 1.0 over the examined thickness range, which explains the low mobility of thinner films by higher energetic disorder.

This analysis proves to be highly advantageous as it represents the whole transfer curve, gives better comparability and offers more physical insight. Our study demonstrates the crucial role of layer thickness tuning for improved film structure and optimum material performance.

DS 26.8 Wed 11:30 H37

Deposition of P3HT via dip coating onto transistors with channel lengths below 1 μm — •Silviu Botnarash, Steve Pittner, and Veit Wagner — School of Engineering and Science, Jacobs University Bremen, Campus Ring 1, D-28759, Germany

A high quality interface between the organic semiconductor and the oxide is crucial for the high performance of an OFET. A good surface treatment is imperative, but it will lower the surface energy of the oxide, making it difficult to spin coat on it uniform semiconductor layers from solvents like chloroform or toluene. We report on the usage of the dip coating technique to achieve highly ordered layers of regioregular poly(3-hexylthiophene) (rr-P3HT). By varying the removal speed of the silicon substrate from solution, the concentration of the solution or both, one can achieve ultrathin layers of rr-P3HT which permit to analyze OFET properties in the sub-monolayer regime. Decreasing the channel length of the transistors down to the range of the contour length of the rr-P3HT is expected to improve the characteristics of the OFET's. An additionally applied electric field between the source and drain electrodes during dip coating facilitates the trapping of P3HT molecules on the electrodes increasing the performance of the device. We used rr-P3HT with an average contour length of 80-100 nm. Compared to previously reported results for chloroform based solutions, the same concentration range of rr-P3HT in toluene displayed better characteristics, which is believed to be due to lower evaporation rate of toluene. Subsequent drying in a nitrogen rich atmosphere over a period of up to 24 h positively influences the performance of the OFET's.

DS 26.9 Wed 11:45 H37

Semitransparent small-molecule organic solar cells — •Jan Meiss[1], Christian Uhrich[2], Stefan Sonntag[2], Wolf-Michael Gnehr[2], Martin Pfeiffer[2], Karl Leo[1], and Moritz Riede[1] — [1]Institut für Angewandte Photophysik, Technische Universität Dresden, 01062 Dresden, Germany — [2]heliatek GmbH, Liebigstraße 26, 01187 Dresden, Germany

Semitransparent, colourful solar cells are of interest for a wide range of applications, e.g. sun shading of residential and office buildings or cars. Previously, among organics-containing devices, only semitransparent dye-sensitized solar cells showed power conversion efficiencies (PCE) that allowed first meaningful applications, whereas semi-transparent small-molecule organic solar cells (OSC) were limited to PCE well below 1%.

We present small-molecule semitransparent OSC deposited by thermal vacuum evaporation on ITO-coated glass. The organic materials include absorber materials and doped dedicated charge transport layers. Due to our unique device architecture, the top electrode is ITO-free, consisting only of an ultra-thin multi-layer metal film.

The OSC exhibit light transmission in the visible range of 30-50% with PCE of over 2%. Organic capping layers are used to significantly lower reflection and increase transmission without significant loss of PCE. Furthermore, we have achieved first large-area semitransparent tandem OSC with 3.5% PCE at 20-40% transmission in the visible range on 4cm^2, which show the potential of this type of device for large-scale building integration.

DS 26.10 Wed 12:00 H37

Stability optimisation of small molecule organic solar cells — •Martin Hermenau, Karl Leo, and Moritz Riede — Institut für Angewandte Photophysik, George-Bähr-Str. 1, 01069 Dresden

In addition to high efficiency and low cost, a long device lifetime is a crucially important factor for the commercialisation of small molecule organic solar cells. Previous results mostly covered unencapsulated devices and showed low lifetimes under 1000 hours even without permanent illumination.

Here, we present results on improving the intrinsic stability of glass-glass-encapsulated p-i-n solar cells containing small molecules. Zinc-Phthalocyanine and the fullerene C_{60} are used as photoactive materials. Doped layers of wide gap materials and C_{60} are used as hole and electron transport layer, respectively. All devices are illuminated with monochromatic or white LEDs and IV characteristics are automatically recorded during the entire measuring period.

In contrast to polymer solar cells, we do not observe an influence of different types of top contact materials on the lifetime. All variations of Gold, Silver and Aluminium lead to stable cells for about 1500 hours of continued illumination.

However, by changing the type and even the thickness of the hole transport material we are able to enhance the extrapolated lifetime (t80) from about 1100 hours with 30nm PV-TPD up to more than 5000 hours with 60nm Di-NPB. These results are achieved with encapsulated devices and illumination intensitites up to 840 mW/cm^2 from high-power white LEDs at controlled temperatures of 50°C.

DS 26.11 Wed 12:15 H37

Self organized molecular electronic junctions using two phase liquid structures in microfluidic channels — •Shashi Thutupalli[1], Mark Elbing[2], Matthias Fischer[2], David Muñoz[3], Ralf Seemann[1,4], Marcel Mayor[2,3], and Stephan Herminghaus[1] — [1]MPI for Dynamics and Self Organization, Göttingen, Germany — [2]Forschungszentrum Karlsruhe GmbH, Institute for Nanotechnology, Karlsruhe, Germany — [3]University of Basel, Department of Chemistry, Basel, Switzerland — [4]Experimental Physics, Saarland University, Saarbrücken, Germany

Using a combination of microfluidics and molecular design, we demonstrate self assembled, reconfigurable molecular electronic junctions. To construct metal-molecule-metal junctions, we employ liquid mercury as the electrode contact in crossed microfluidic channels. Self assembled monolayers (SAM's) of conducting molecular rods are created on the surface of the mercury, which are then bridged to the other mercury electrode via microfluidic control. By precise flow control, we create rectifying molecular junctions using asymmetric molecules. We report on the electrical properties of these microfluidic metal-molecule-metal junctions. Also, we use surfactant stabilized foam-like water-in-oil emulsions to form variable molecular junctions. Here, molecules synthesized with hydrophobic conducting cores and hydrophilic ends self-insert into the lamellae between aqueous droplets. Using the aqueous droplets then as the molecular contacts, we report on the conducting properties of the inserted molecules and demonstrate the possibility of reconfigurable circuits using topological droplet rearrangements.

DS 26.12 Wed 12:30 H37

DNA Based Molecular Electronics Using Mercury Droplets in Microfluidic Channels — •Shuang Hou, Shashi Thutupalli, and Stephan Herminghaus — Max Planck Institute for Dynamics and Self Organization, D-37073, Göttingen, Germany

Mercury droplets in microfluidic channels are used as electrodes to investigate the electronic properties of single strand DNA (ssDNA) molecules. In this system, a self assembled monolayer (SAM) of thiolated DNA oligomers (~ 5 nm length) of specific base sequences is formed on the surface of mercury droplets. Two such droplets are then brought together by microfluidic manipulation to form a mercury-ssDNA-mercury electrical junction. We identified single SAMs of ssDNA oligos, double SAMs of ssDNA oligos of the same composition, and complementary binding DNA composed junctions. Here, we report the influence of base pair type and DNA sequence length to the electronic characteristics. On the basis of these results, the design of DNA based molecular electronic elements (such as diodes) seems possible.

DS 27: [O] Plasmonics and Nanooptics III (Joint Session DS/O/HL)

Time: Wednesday 10:30–13:15 Location: H32

DS 27.1 Wed 10:30 H32

3D optical Yagi-Uda nanoantenna array — •Daniel Dregely, Richard Taubert, and Harald Giessen — University of Stuttgart, Germany

Optical nanoantennas have gained a lot of interest in the past few years [1,2]. They are able to link propagating radiation and confined optical fields. Only little work has been done on complex antenna geometries on the nanoscale. In our experiments, we investigate a 3D optical Yagi-Uda nanoantenna array. Due to the high directivity of the array structure the incoming light is received efficiently at resonant wavelengths in the near-infrared (around $\lambda = 1.3$ μm).

Our 3D gold nanoantenna structure was fabricated with electron beam lithography using layer-by-layer stacking. We measured the transmission and reflection spectra of the nanoantenna array from both directions in order to examine the directive behavior of the structure. FIT-calculations agree very well with our experimental findings and confirm the concentration of the incoming plane-wave radiation to the feeding points of the antenna array.

References: [1] P. Mühlschlegel, H.-J. Eisler, O. J. F. Martin, B. Hecht, and D. W. Pohl, Science 308, 1607 (2005). [2] T. H. Taminiau, F. D. Stefani, F. B. Segerink, and N. F. van Hulst, Nature Photon. 2, 234 (2008).

DS 27.2 Wed 10:45 H32

Few-cycle nonlinear optics of single plasmonic nanoantennae — •Tobias Hanke, Günther Krauss, Daniel Träutlein, Barbara Wild, Rudolf Bratschitsch, and Alfred Leitenstorfer — Department of Physics and Center for Applied Photonics, University of Konstanz, D-78457 Konstanz, Germany

We have studied the nonlinear optical properties of single gold nanoantennae driven with few-cycle laser pulses in the near infrared [1]. Intense third harmonic emission is obtained when exciting with fundamental spectra below 1.1 eV. At higher photon energies frequency doubling and two-photon induced luminescence are observed. We relate these findings to the band structure of bulk gold, especially a two-photon resonance with the d-band transitions.

The intense third-harmonic emission enables precise detection of frequency-resolved interferometric autocorrelation traces of individual nanoantennae. We find an enhancement up to 3 orders of magnitude when driving on resonance with the fundamental plasmon mode. A sub-cycle dephasing time as short as 2 fs is measured directly in the time domain, highlighting the strong radiation coupling and ultrabroadband response of these efficient nanodevices.

[1] Hanke et al., Phys. Rev. Lett., accepted for publication.

DS 27.3 Wed 11:00 H32

plasmon-enhanced high-order harmonic generation in the vicinity of metal nanostructures — •song-jin im, anton husakou, and joachim herrmann — Max-Born-Institute for Nonlinear Optics and Short Pulse Spectroscopy, Max-Born-Str. 2a, D-12489 Berlin, Germany

Generation of high harmonics in noble gases is one of key topics of nonlinear optics, which is of a critical importance in many disciplines, for example in attosecond physics. Recently, plasmon-enhanced high-order harmonic generation became possible in the vicinity of bow-tie shaped nanostructures by pulses directly from an oscillator with MHz repetition rate. In this contribution, we simulate high-order harmonic generation by sub-TW/cm^2 pulses using large plasmon field enhancement near metallic nanostructures such as bowtie-shaped antennas or nanocones. Our simulations using a commercial software JCMwave predict intensity enhancement of 3 orders of magnitude near the surface of silver nanocones. The generation of the high harmonics was modeled using a modified Lewenstein approach taking into account the inhomogeneity of the field and the electron absorption by the metal. Our results are consistent with experimental observations for bowtie elements. Considering the generation of high harmonics in argon in the vicinity of silver nanocones, we show that harmonics numbers up to 50, corresponding to 15 nm wavelength, can be achieved using relatively low input intensity of 300 GW/cm^2, characteristic for nJ laser pulses directly from a laser oscillator with MHz repetition rate.

DS 27.4 Wed 11:15 H32

Analytic photoemission localization and switching in plasmonic nanoantennas by laser pulse shaping — Martin Aeschlimann[1], Michael Bauer[2], Daniela Bayer[1], Tobias Brixner[3], Stefan Cunovic[4], Alexander Fischer[1], Pascal Melchior[1], Walter Pfeiffer[4], Martin Rohmer[1], Christian Schneider[1], Christian Strüber[4], •Philip Tuchscherer[3], and Dmitri V. Voronine[3] — [1]Fachbereich Physik and Research Center OPTIMAS, Technische Universität Kaiserslautern, Erwin-Schrödinger-Str. 46, 67663 Kaiserslautern, Germany — [2]Institut für Experimentelle und Angewandte Physik, Universität Kiel, Leibnizstr. 19, 24118 Kiel, Germany — [3]Institut für Physikalische Chemie, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany — [4]Fakultät für Physik, Universität Bielefeld, Universitätsstr. 25, 33615 Bielefeld, Germany

We experimentally achieve two-photon photoemission localization and switching on a subwavelength scale in plasmonic nanoantennas. Complex polarization-shaped laser pulses which are found in adaptive optimizations control the linear response of the nanostructure. We consider previous analytic investigations to identify the interference of two excited modes in the nanostructure as the main control mechanism. The optimal pulse shapes for switching are then found deterministically. Adaptive and analytic control schemes are compared, and agreement between both approaches is demonstrated.

DS 27.5 Wed 11:30 H32

Swichable Hot Spots in Bipyramid-Nanoresonators — •Siji Wu, Calin Hrelescu, Frank Jäckel, and Jochen Feldmann — Photonics and Optoelectronics Group, Department of Physics and Center for Nano Science (CeNS), Ludwig-Maximilians-Universität München, Amalienstrasse 54, 80799 München, Germany

Highly enhanced and strongly localized electromagnetic fields, so-called hot spots, are attractive for imaging applications, based on raman scattering or fluorescence enhancement.[1,2] Hot spots can be provided by nonspherical gold nanoparticles or nanoparticles aggregates. Here, we report on nanoresonators consisting of two bipyramidal gold nanoparticles prepared by AFM manipulation. Applying a force with the AFM allows switching between the two possible adsorption geometries of an individual bipyramid on the substrate. The plasmonic coupling between two bipyramids is different in the two configurations. Consequently, the hot spot in the nanoresonator can be switched mechanically. Furthermore, the hot spot can be located within 1nm above the substrate surface in contrast to dimer nanoresonators from spheres, rods or ellipsoids.

[1] C. Hrelescu, T.K. Sau, A.L. Rogach, F. Jäckel, J. Feldmann Appl. Phys. Lett., 94, 153113 (2009)

[2] A. Bek, R. Jansen, M. Ringler, S. Mayilo, T. A. Klar, J. Feldmann Nano Lett., 8 (2), 485 (2008)

DS 27.6 Wed 11:45 H32

Near-field measurements on nanoscopic sphere-on-plane-systems by means of PEEM — •Florian Schertz[1], Marcus Schmelzeisen[2], Hans-Joachim Elmers[1], Gerd Schönhense[1], and Max Kreiter[2] — [1]Inst. f. Physik, Johannes Gutenberg-Universität, 55099 Mainz — [2]Max-Planck-Inst. f. Polymerforschung, 55128 Mainz

Surface immobilized gold nano-spheres above a gold surface with a gap distance in the order of a nanometer act as sphere-on-plane (SOP) optical resonator systems showing unique optical properties. In the vicinity of a flat metal surface, a second resonance band red-shifted with respect to the isolated particle resonance occurs, understandable on the basis of multipole interactions of the sphere with its own mirror image in the gold film. Several theoretical and optical far-field studies of SOP resonators were performed, investigating the dependence of the resonance wavelength on the resonator geometry and dielectric properties of the spacer material [1]. The optical near-field of the system under fs-laser-radiation causes highly non-linear (n=3-5) photoemission processes strongly varying depending on the particle properties. Photoelectron microscopy turned out to be a valuable tool for the investigation of the optical near-field of individual SOPs (cf.[2]). We present the gap-resonance-induced photoemission characteristics of several SOPs (individually characterized by SEM), excited by fs-laser radiation in the range from 750nm to 850nm. This work was supported by DFG (EL172-16) and MWFZ, Univ. Mainz. [1] A. Rueda et al., J. Phys. Chem. C 112 (2008) 14801, and Refs. therein. [2] M. Cinchetti et al., Phys. Rev. Lett. 95 (2005) 047601

DS 27.7 Wed 12:00 H32

Strong-field photoelectron emission from metal nanotips — •Max Gulde, Reiner Bormann, Alexander Weismann, Sergey Yalunin, and Claus Ropers — University of Göttingen, Courant Research Center Nano-Spectroscopy and X-Ray Imaging, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

The generation of ultrashort, localized electron pulses is of fundamental interest for future applications in time-resolved electron imaging and diffraction. Femtosecond electron sources of great spatial coherence make use of a combination of local field enhancement at metal nanotips and nonlinear photoelectric effects. Previous studies have resulted in a controversial debate about the underlying physical processes.

Here, we present our most recent theoretical and experimental results regarding ultrafast photoelectron emission from nanometric gold tips. For the first time, we conclusively show the transition between the multiphoton and the optical field emission (i.e. tunneling) regimes. Direct evidence for this transition is found from both the power dependence of the total current and the spatial characteristics of the resulting electron beam. The results are supported by theoretical modeling.

DS 27.8 Wed 12:15 H32

Dark-Mode Plasmonic Nanorod Cavity — •Johannes Kern, Swen Grossmann, Jer-Shing Huang, Paolo Biagioni, and Bert Hecht — Experimental Physics 5, University of Würzburg, Germany

We report ultra-small nanoplasmonic cavities consisting of a self-assembled, side-by-side aligned gold nanorod dimer. The rods are 50-70 nm long and are separated by a 3 nm gap. The structure corresponds to a finite piece of a two-wire transmission line with two highly reflective open ends which supports a quasi-TE fundamental mode which propagates along the transmission line. Reflection at the end caps leads to length-dependent Eigenmodes, whose energies are determined by the cavity length and the phaseshift introduced upon reflection. Unlike the dipolar longitudinal and transverse plasmon resonances that are also supported by the structure, the fundamental cavity mode is a dark quadrupol mode.

Nevertheless the cavity mode is experimentally accessible by excitation of electron-hole pairs in the gold bandstructure, which act as local dipole sources. The ultra-small mode volume and comparatively high Q-factor leads to a high selectivity of the cavity and the electron-hole pairs preferentially decay into the cavity resonance. Therefore luminescence spectra of the cavities clearly show the peak of the cavity mode. The wavelength of the cavity mode depends on the cavity length and lies in the VIS region, consistent with FDTD simulations and analytical modeling.

The ultra-small mode volume and high Q-factor make our cavities promising candidates to study lasing and/or strong coupling effects.

DS 27.9 Wed 12:30 H32

Temperature related nanoantenna extinction in infrared range — •Chung Hoang, Frank Neubrech, Makus Klevenz, Robert Lovrincic, Olaf Skibbe, and Annemarie Pucci — Kirchhoff-Institut für Physik der Universität Heidelberg, Im Neuenheimer Feld 227, 69120 Heidelberg

We present important progress in the experimental studies of single-crystalline lead nanorods grown on Si(557) vicinal surfaces by self-assembling process in ultra-high vacuum. The growth of such nanorod arrays is governed by four experimental parameters: substrate temperature, surface energy, deposition rate, and amount of deposited lead. Upon cooling, strong enhancement of the infrared signal at resonance is observed, indicating the increase of extinction-cross section. This scenario can be attributed to the reduction of electron scattering events where electron - phonon scattering is the main factor that is involved in this process. Below half of the Debye temperature, the maximum resonant antenna extinction is nearly temperature independent, indicating residual electron scattering at surfaces.

DS 27.10 Wed 12:45 H32

Polarization-independent chiral split-ring resonator arrays with colossal optical activity — •Max Wunderlich, Sebastian Engelbrecht, Alexey Shuvaev, and Andrei Pimenov — Experimentelle Physik IV, Universität Würzburg

We have studied the optical activity of bi-layered split-ring resonator arrays. They form chiral quasi-molecules due to inductive coupling. We have examined these structures with the instruments of quasioptical terahertz-spectroscopy. Our investigation shows that such systems can produce a colossal optical activity of 600 degree per wavelength. This results might lead to negative refraction due to chirality. Furthermore we present a way to effectively suppress polarization-dependent behavior of split-ring resonator arrays by introducing C_n symmetries. Thus we have demonstrated a way to realize a ultra-thin orientation-independent polarization rotator.

DS 27.11 Wed 13:00 H32

Efficient surface-plasmon-polariton excitation on nanoparticle structures by inclined incident light — •Andreas Seidel, Wei Cheng, Andrey Evlyukhin, Carsten Reinhardt, and Boris Chichkov — Laser Zentrum Hannover e.V., Hollerithallee 8, 30419 Hannover

We study the features of local surface plasmon polariton (SPP) excitation on single and chains of gold nanoparticles positioned near a gold surface using a light beam under inclined incidence. It is shown that by tuning the incident angle and the parameters of the surface nanoparticle structure one could obtain symmetric or asymmetric excitations of SPP beams propagating along certain directions depending on the particle/chain distances. The reasons and conditions for this behaviour and efficiency of SPP excitation as a function of the incident angle are studied. It is demonstrate that the SPP excitation efficiency strongly depends on the incident angle. Adjusting the incident angle to the maximum field component perpendicular to the metal dielectric interface can lead to a large increase of SPP excitation efficiency. In the case of nanoparticle chains the symmetric or asymmetric patterns of the SPP distributions are the result of the interference of the scattered waves generated by each nanoparticle in a structure. The theoretical consideration is based on the Green*s function technique for the Maxwell equations of the total electric field and on the point-dipole approximation. Experimental investigation is realized by leakage radiation microscopy in real and reciprocal space.

DS 28: [O] Plasmonics and Nanooptics IV (Joint Session DS/O/HL)

Time: Wednesday 15:00–17:45 Location: H32

DS 28.1 Wed 15:00 H32

Raman and Luminescence Enhancement Produced in Gap-mode Near-field Optical Microscopy — •Dai Zhang, Marcus Sakrow, Kai Braun, and Alfred J. Meixner — Institute of Physical and Theoretical Chemistry, University Tübingen, Auf der Morgenstelle 8, Tübingen

Tip-enhanced near-field optical microscopy can produce spectroscopic images of molecular layers deposited on smooth Au-surfaces, of single molecules and of organic semi-conductor films with an optical resolution on the order of 10 nm. This is made possible by a sharp laser-illuminated Au-tip approaching as close as a few nanometers to the sample surface. The system behaves as an optical antenna for confining and enhancing the excitation field to a small sub-diffraction volume in the gap between the tip-apex and the surface and retrieving emitted or scattered photons to the far field for detection. In this way the signal emitted from the gap can be enhanced by several orders of magnitude with respect to the diffraction limited background signal by enhancing the excitation efficiency and the emission yield. In this contribution, a variety of enhancement mechanisms will be discussed.

DS 28.2 Wed 15:15 H32

Quantifying Excitation and Radiation Rate Enhancement Provided by Near-field Optical Antennas — •Miriam Böhmler, Nicolai Hartmann, Carsten Georgi, and Achim Hartschuh

— Department Chemie und Biochemie & CENS, Ludwig-Maximilians-Universität, 81377 München

Tip-enhanced near-field optical microscopy provides nanoscale optical resolution beyond the diffraction limit [1]. This is due to the highly confined enhancement of the optical fields at the tip apex, which locally increases both excitation and radiation rates. In our experiments we use sharp gold tips to probe the photoluminescence (PL) of individual single-walled carbon nanotubes. We show that excitation and emission enhancement can be distinguished by imaging the radiation pattern in the back focal plane of the microscope objective. The analysis is based on the characteristic radiation patterns generated by single dipoles with a particular orientation in 3D [2]. We first find that the PL emission of a nanotube can be described by an in-plane oriented dipole. In the presence of our tip, the radiation pattern is strongly modified and dominated by the signatures of a vertical dipole corresponding to the tip axis. This observation illustrates the spatial redirection of the emission by the tip acting as an optical antenna [3]. By comparing radiation patterns with and without the influence of our tip, we estimate excitation and radiation rate enhancement quantitatively.

[1] A. Hartschuh, Angew. Chem. Int. Ed. 47, 8178 (2008)

[2] M. A. Lieb, J. Opt. Soc. Am. B 21, 1210 (2004)

[3] T. H. Taminiau, Nat. Photon. 2, 234 (2008)

DS 28.3 Wed 15:30 H32

Pseudo-heterodyne scanning near-field optical microscope for surface plasmon detection with actively stabilized phase — •Stefan Griesing, Andreas Englisch, and Uwe Hartmann — Experimental Physics, Saarland University, D-66123 Saarbrücken

Amplitude and phase of the evanescent surface plasmon field were detected by a pseudo-heterodyne scanning near-field optical microscope (SNOM). Light from a HeNe laser (l = 633nm) and an argon ion (Ar) laser (l = 488nm) was combinied in a fiber coupler. One output channel of the coupler served as reference branch of an interferometer. A piezoelectric fiber stretcher in that branch was used for sinusoidal phase modulation. The other output of the coupler was linked to another coupler. By using different color filters, the two wavelengths were separated at the output channels. The HeNe laser was used for surface plasmon excitation under attenuated total internal reflection. The light from the Ar laser illuminated the sample under normal incidence, so that during the scanning process a constant phase from the Ar laser was detected. The SNOM tip detects both, surface plasmons excited by the HeNe laser and the spot from the Ar laser. The signal is combined in a third fiber coupler with the signal from the reference branch. At the output, the interference signal was wavelength- selectively detected by Si photodiodes and lock-in amplifiers. The signal from the Ar laser was used as input for a feedback- loop which modifies the drive signal of the fiber stretcher. In this way, the phase fluctuations due to thermal and mechanical disturbances were compensated.

DS 28.4 Wed 15:45 H32

Scattering near-field microscopy in the THz with a free-electron laser — •Hans-Georg von Ribbeck[1,2], Marc Tobias Wenzel[1], Rainer Jacob[2], and Lukas M. Eng[1] — [1]Institut für Angewandte Photophysik, TU Dresden, 01062 Dresden, Germany — [2]Institut für Ionenstrahlphysik und Materialforschung, Forschungszentrum Dresden - Rossendorf, 01314 Dresden

We present scattering-type scanning near-field optical microspectroscopy (s-SNOM) invstigations, successfully operated in the THz range with a wavelength independent spatial resolution of 150 nm. Our microscopy set-up bases on a true noncontact atomic force microscope (nc-AFM) combined with the free-electron laser (FEL) source at the Forschungszentrum Dresden-Rossendorf. This laser provides tunability from 30 - 250 um. We were able to record, for the first time ever, s-SNOM signatures with a FEL at wavelengths ranging from 30 um to 180 um (10 - 1.67 THz). In addition to the near-field dependent optical signals we also demonstrate the imaging capabilities of our THz-s-SNOM. Image scans were performed on a specially designed test structure consisting of a topography-free composite of a polymer/gold sample. On such samples, topography independent strong optical material contrast could be demonstrated at 150 um wavelength. We achieve a resolution of better than 150 nm corresponding to better than l/1000.

DS 28.5 Wed 16:00 H32

Ultrahigh temporal and spatial resolution imaging of second harmonic fields in random zinc oxide nanostructure arrays — •Manfred Mascheck[1], Slawa Schmidt[1], Martin Silies[1], Takashi Yatsui[2], Motoichi Ohtsu[2], David Leipold[3], Erich Runge[3], and Christoph Lienau[1] — [1]Carl-von-Ossietzky-Universität, Oldenburg — [2]University of Tokyo — [3]Technische Universität Ilmenau

Among the most prominent signatures of the weak (Anderson) localization of light in random dielectric media are an enhanced coherent backscattering and the localization of electromagnetic fields in both space and time. Light localization is particulary relevant in nanophotonic materials, where it can give rise to strong field localization and greatly enhanced optical nonlinearities.

Here, we explore this light localization in densely packed, random arrays of ZnO nanoneedles with tip diameters of less than 20 nm. A phase-stabilized pair of 6 fs laser pulses is focused to its diffraction limit of $1\,\mu m^2$ onto the ZnO needles.

The generated surface second harmonic (SH) spectra are detected as a function of the lateral position of the laser focus and the delay between the two pulses. We observed a pronounced spatial localization of the SH signal in hot spots of less than 300 nm dimension. We show, by retrieving the time structure of the localized electric field from interferometric FROG traces, that light is stored in these hot spots for more than 100 fs. Such nanoneedle arrays therefore present a highly interesting new model system for exploring the rich physics of weakly localized light fields.

DS 28.6 Wed 16:15 H32

Second Harmonic Imaging of Gold Nanocones with a Parabolic Mirror Microscope — •Anke Horneber[1], Dai Zhang[1], Monika Fleischer[2], Marcus Sackrow[1], Kai Braun[1], Dieter P. Kern[2], and Alfred J. Meixner[1] — [1]Institute of Physical Chemistry, Eberhard Karls University Tübingen, Germany — [2]Institute of Applied Physics, Eberhard Karls University Tübingen, Germany

Second harmonic generation (SHG) is a valuable technique for the visualization of surfaces. Our confocal optical microscope uses a parabolic mirror with a smaller focus than objective lenses in air and the largest possible signal collection angle. We use higher order laser modes which are often called cylindrical vector beams for the investigation of complex plasmonic structures. The longitudinal polarization component in a radially polarized laser beam focus can excite the longitudinal plasmon of a gold cone most efficiently[1]. We present first SHG images of gold nanocones with an optical resolution below 300 nm. We are developing a flexible setup that will allow non-linear experiments as well as near-field measurements. Such a setup will provide further opportunities like non-linear near-field investigations and the combination of a high spatial resolution with ultrafast dynamics.

[1] M. Fleischer et al., APL, 93 (2008) 111114.

DS 28.7 Wed 16:30 H32

Nanosphere Lithography of Sub-50 nm Plasmonic Structures — •Jun Zhao, Bettina Frank, and Harald Giessen — Universität Stuttgart, Deutschland

Nanosphere lithography is a powerful and fast fabrication technique for periodic large-area metallic nanostructures of different and complex shapes [1]. We use tilted-angle-rotation thermal evaporation onto the monolayers of close-packed polystyrene nanospheres to fabricate metamaterial samples of up to $1cm^2$.

With this fabrication technique we can prepare sub-50 nm plasmonic structures such as pentamers, hexamers, and also ring structures with a centered or off-centered disk in the middle, which is useful for investigation of Fano-type plasmon resonances and future sensors.

The optical response of our structures was measured in reflectance geometry with FTIR-microscopy. The measurements show good agreement with our simulations. We also performed stacking experiments of split-ring resonators, which can be arranged in an ordered or twisted stereometamaterial fashion [2].

[1] . M. C. Gwinner, E. Koroknay, L. Fu, P. Patoka, W. Kandulski, M. Giersig, and H. Giessen, Small 5, 400 (2009) [2]. N. Liu, H. Liu, S. Zhu, and H. Giessen, Nature Photonics 3, 157 (2009)

DS 28.8 Wed 16:45 H32

Gold nanocone probes for near-field scanning optical microscopy — •Bastian Zeeb, Christian Schäfer, Peter Nill, Monika Fleischer, and Dieter P. Kern — Institute of Applied Physics, University of Tübingen, Auf der Morgenstelle 10, 72076 Tübingen

Apertureless near-field scanning optical microscopy (ANSOM) provides the possibility to collect simultaneously high-resolution topographical and sub-diffraction limited optical information from a surface. When optically excited, the scanning probes act as optical antennae with a strong near-field enhancement near the tip apex. Spatial resolution and optical near-field enhancement depend strongly on the properties and geometry of the scanning probe - in particular on very sharp tip radii. Various possibilities for fabricating good antennae have been pursued. Most commonly, scanning probes consist of electrochemically etched gold wires which are sharp but not well-defined in geometry.

We present two different approaches for ultra sharp and well-defined antennae based upon fabricating gold nanocones with a tip radius smaller than 10 nm which can be used in ANSOM [e.g. *M. Fleischer et al., Appl. Phys. Lett. **93**, 111114 (2008)*]. A transfer process is presented that can be used to attach single gold nanocones to non-metallic probes such as sharp glass fiber tips. Alternatively, new processes are presented to fabricate cones directly on pillars of different materials such as silicon or bismuth, which can be applied to cantilever tips for ANSOM scanning applications.

DS 28.9 Wed 17:00 H32

Space Charge Effects in Photoemission Electron Microscopy — •Jan Vanis, Niemma M. Buckanie, Ping Zhou, Dietrich von der Linde, Michael Horn-von Hoegen, and Frank-J. Meyer zu Heringdorf — University Duisburg-Essen, Germany

We use the combination of a spectroscopic Photoemission Electron Microscope (PEEM) with femtosecond (fs) laser pulses to investigate samples with high spatial and temporal resolution. For proper imaging, the laser pulses must have sufficiently low intensity to minimize the space charge. Here, we report on experiments with a regenerative Ti:sapphire amplifier system. The laser setup generates fs-pulses ($\lambda = 800\ nm$, i.e., a photon energy of $E = 1.55\ eV$). The system has a variable repetition rate up to 250 kHz. We studied Ag islands which have been grown *in-situ* by self-assembly on Si(111) surfaces. We used the fundamental and the 4th harmonic ($E = 6.2\ eV$) of the amplifier system to evaluate space charge effects in PEEM. The space charge effect is reflected in an energetic broadening of the electron distribution and, at higher laser fluence, in a loss of focus. Insertion of apertures into the electron path provides a way to change the electron density in different areas of the microscope and locate in which section of the PEEM the space charge effect is dominant. The influence of the laser energy, wavelength, and repetition rate on the energy spectra and the image distortions will be discussed.

DS 28.10 Wed 17:15 H32

Characterization of Single Gold Nanoparticles Using Confocal Interference Microscopy in Combination with Higher Order Laser Modes — •Frank Wackenhut[1], Tina Züchner[1], Antonio Virgilio Failla[1,2], and Alfred J. Meixner[1] — [1]Eberhard-Karls-Universität Tübingen, Institut für Physikalische und Theoretische Chemie, Tübingen, Germany — [2]Max-Planck-Institut für Entwicklungsbiologie, Tübingen, Germany

By using confocal interference microscpoy in combination with higher order laser modes it is possible to directly image the orientation and to detect the shape of single metal nanoparticles, with sizes well beyond the diffraction limit [1,2]. Metal nanoparticles can be imaged by detecting both their luminesence or the elastically scattered light. In the scattering detection mode the visualized pattern strongly depends on the local environment, e.g. the refractive index of the surrounding medium [3]. With this technique we are also able to observe and quantify dynamics in the motion of single nanoparticles [4]. Ongoing measurements show that this technique might be utilized for studying the wavelength dependence of the polarizability tensor of a single gold nanorod.

[1] A.V. Failla, H. Qian, H. Qian, A. Hartschuh, A. J. Meixner (2006), Nano Lett. 6, 1374. [2] T. Züchner, A. V. Failla, A. J. Meixner (2008), J. Microsc. 229, 337. [3] T. Züchner, A. V. Failla, M. Steiner, A. J. Meixner (2008), Opt. Expr. 16, 14635. [4] T. Züchner, F. Wackenhut, A. V. Failla, A. J. Meixner (2009), Appl. Surf. Sci. 255, 5391.

DS 28.11 Wed 17:30 H32

Polarization dependence of the optical response of individual metallic nanostructures and arrays — •Reto Giannini[1], Yasin Ekinci[1,2], and Jörg F. Löffler[1] — [1]Laboratory of Metal Physics and Technology, Department of Materials, ETH Zurich, 8093 Zurich, Switzerland — [2]Laboratory of Micro and Nanotechnology, Paul Scherrer Institute, 5232 Villigen PSI, Switzerland

The optical response of designed metallic nanostructures depends strongly on the properties of the exciting light beam, and especially on the polarization relative to the characteristic axis of the nanostructures. To address this dependence, we established an experimental setup in the visible wavelength range that allows us to measure the optical response of individual metallic nanostructures and arrays with varying incident wave vectors and polarization. The possible excitation covers the whole range from normal excitation (relative to the surface of the substrate) to parallel excitation. The latter is realized using objective-based TIRF. In this presentation, we explain the principle of our setup and the optical response of various Au-nanostructures, such as pillars and dimers under varying wave vectors and polarization.

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

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

DS 29.1 Wed 15:00 Poster A

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

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

DS 29.2 Wed 15:00 Poster A

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

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

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

DS 29.3 Wed 15:00 Poster A

Spectroelectrochemical Characterization of Thin Films of Hexadecafluorophthalocyaninatozinc Prepared by Vapour Deposition

— •Mareike Falk, Stefanie Nagel, Christopher Keil, and Derck Schlettwein — Institute of Applied Physics, Justus-Liebig-University Giessen, Germany. email:schlettwein@uni-giessen.de

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

DS 29.4 Wed 15:00 Poster A

Model supported generation of Reflection Anisotropy Spectra of copper phthalocyanine films on isotropic and anisotropic silicon substrates

— •Falko Seidel, Li Ding, and Dietrich R. T. Zahn — Semiconductor Physics, Chemnitz University of Technology, D-09107 Chemnitz, Germany

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

DS 29.5 Wed 15:00 Poster A

Influence of electric and magnetic fields during film growth of phthalocyanines

— •Florian Latteyer[1], Vladimir Plyashkevich[2], Tamara Basova[2], Heiko Peisert[1], and Thomas Chassé[1] — [1]University of Tübingen, Institute for Physical and Theoretical Chemistry, Tübingen, Germany — [2]Nikolaev Institute of Inorganic Chemistry, Novosibirsk, Russia

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

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

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

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

DS 29.6 Wed 15:00 Poster A

In-situ Optical Spectroscopy During the Growth of Phthalocyanine Thin Films on Single Crystalline Substrates

— •Enno Lorenz[1], André Dragässer[1], Christopher Keil[1], Jens Wallys[2], Martin Eickhoff[2], and Derck Schlettwein[1] — [1]Institute of Applied Physics, Justus-Liebig-University Giessen, Germany. email:schlettwein@uni-giessen.de — [2]Experimental Physics I, Justus-Liebig-University Giessen, Germany.

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

DS 29.7 Wed 15:00 Poster A

Structure optimization of pentacene thin film transistors controlled by substrate temperature and annealing

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

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

DS 29.8 Wed 15:00 Poster A

Trap-state influence on charge carrier transport in perylene based OTFTs

— •Christian Effertz, Ingolf Segger, Philip Schulz, and Matthias Wuttig — Institute of Physics (IA), RWTH Aachen University of Technology, 52056 Aachen, Germany

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

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

DS 29.9 Wed 15:00 Poster A

Tailoring ferroelectric interfaces: surface modification of PZT mediated through functionalized thiophene derivates

— •Peter Milde[1], Kinga Haubner[2,3], Evelyn Jähne[3], Denny Köhler[1], Ulrich Zerweck[1], and Lukas M. Eng[1] — [1]Department of Applied Photophysics, TU Dresden, Dresden, Germany — [2]Leibniz Institute for Solid State and Materials Research Dresden, TU Dresden, Dresden, Germany — [3]Institute of Macromolecular Chemistry and Textile Chemistry, TU Dresden, Dresden, Germany

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

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

DS 29.10 Wed 15:00 Poster A

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

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

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

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

DS 29.11 Wed 15:00 Poster A

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

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

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

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

DS 29.12 Wed 15:00 Poster A

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

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

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

DS 29.13 Wed 15:00 Poster A

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

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

DS 29.14 Wed 15:00 Poster A

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

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

DS 29.15 Wed 15:00 Poster A

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

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

DS 29.16 Wed 15:00 Poster A

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

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

DS 29.17 Wed 15:00 Poster A

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

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

DS 29.18 Wed 15:00 Poster A

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

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

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

DS 29.19 Wed 15:00 Poster A

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

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

DS 29.20 Wed 15:00 Poster A

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

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

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

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

DS 29.21 Wed 15:00 Poster A

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

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

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

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

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

DS 29.22 Wed 15:00 Poster A

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

As a new technology in light sources the organic light-emitting diodes (OLEDs) have improved rapidly in recent years. One of the remaining challenges is to enhance light outcoupling. Especially the excitation of waveguide modes (WGMs) inside the organic layers and surface plasmons (SPs) at the interface to the cathode strongly reduce the efficiency. These loss channels usually are not accessible for a profound analysis. Therefore, we investigate a simplified OLED stack consisting of only a glass substrate, a metallic silver layer and Alq_3 (tris-(8-hydroxyquinoline) aluminum). In this stack it is possible to extract and measure WGMs as leaky modes and to couple out SPs by a reversed Kretschmann configuration. The occurrence and extraction of WGMs and SPs is studied in detail by varying the thickness of the silver and the Alq_3 layer and by a comparison to numerical simulations. The results obtained in this study offer a deeper understanding of WGMs and SPs, which is a first step to reduce these optical losses and to significantly enhance the efficiency of OLEDs.

DS 29.23 Wed 15:00 Poster A

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

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

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

DS 29.24 Wed 15:00 Poster A

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

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

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

DS 29.25 Wed 15:00 Poster A

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

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

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

DS 29.26 Wed 15:00 Poster A

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

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

DS 29.27 Wed 15:00 Poster A

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

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

DS 29.28 Wed 15:00 Poster A

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

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

DS 29.29 Wed 15:00 Poster A

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

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

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

DS 29.30 Wed 15:00 Poster A

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

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

DS 29.31 Wed 15:00 Poster A

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

Mankind's energy demand is steadily increasing. Novel techniques for environmental friendly energy conversion are therefore a challenging task. Organic solar cells based on donor-acceptor blends present a quite new approach, which posses a large market potential although their efficiency is rather low compared to their inorganic counterparts. In polymer based "bulk heterojunction"-type solar cells so-called "low bandgap" materials are promising donor components in active layers. Low optical bandgap conjugated polymers may improve the efficiency of organic photovoltaic devices by increasing the absorption in the visible and near infrared region of the solar spectrum and by optimizing the offset of the LUMO (lowest unoccupied molecular orbital) energy levels of the donor and acceptor. A potential candidate in this context is Poly[2,6-(4,4-bis-(2-ethylhexyl)-4H-cyclopenta[2,1-b;3,4-b'] dithiophene)-alt-4,7(2,1,3-benzothiadiazole) (PCPDTBT). We study the electronic structure and interface properties to gold and ITO of PCPDTBT by X-ray and UV photoemission spectroscopies (XPS, UPS) as well as X-ray absorption spectroscopy (XAS). The energy level alignment points to charge transfer processes across the interface. In addition, strong chemical interactions occur which may have consequences for interface properties in devices.

DS 29.32 Wed 15:00 Poster A

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

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

DS 29.33 Wed 15:00 Poster A

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

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

DS 29.34 Wed 15:00 Poster A

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

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

DS 29.35 Wed 15:00 Poster A

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

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

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

DS 29.36 Wed 15:00 Poster A

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

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

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

DS 29.37 Wed 15:00 Poster A

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

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

DS 29.38 Wed 15:00 Poster A

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

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

DS 29.39 Wed 15:00 Poster A

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

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

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

DS 29.40 Wed 15:00 Poster A

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

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

DS 29.41 Wed 15:00 Poster A

Formation of palladium hydrides in low temperature Ar/H_2-plasma — •Harm Wulff, Marion Quaas, Heiko Ahrens, Oxana Ivanova, and Christiane A. Helm — University of Greifswald, Institute of Physics, F.-Hausdorff-Str. 6, 17487 Greifswald

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

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

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

DS 29.42 Wed 15:00 Poster A

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

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

DS 29.43 Wed 15:00 Poster A

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

Thin films of doped lanthanum manganites like $La_{0.7}Ca_{0.3}MnO_3$ (LCMO) show a distinctive colossal magneto resistance. In this work we report on x-ray photoelectron diffraction (XPD) measurements of LCMO films (grown by pulsed laser deposition) and of $SrTiO_3$ (STO). The presented polar scans were measured in [100]- and [110]-direction in both cases. In the case of STO the measured polar scans are typical of a cubic crystal structure. In comparison to that the polar scans of LCMO indicate a strained structure.

DS 29.44 Wed 15:00 Poster A

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

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

Therefore, in this study binary Sb-Bi thin films were evaporated in varying stoichiometry and examined structurally (XRD, XRR) and optically (ellipsometry). The binary Sb-Bi system was chosen since these alloys provide three p-electrons per atom throughout, thus fulfilling the prerequisite to be accurately described by the map in every stoichiometry. Additionally, they show a stoichiometric trend regarding the magnitude of the rhombohedral distortion, which is a well know property of some phase-change materials. These trends can be related to a change in the electronic and structural properties, e.g. a varying magnitude of the rhombohedral distortion.

[1] D. Lencer et al., Nature Materials 7, 972 (2008)

DS 29.45 Wed 15:00 Poster A

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

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

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

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

DS 29.46 Wed 15:00 Poster A

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

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

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

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

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

DS 29.47 Wed 15:00 Poster A

Structural optimization of CoFeB/MgO/CoFeB TMR ele-

ments — •Patrick Peretzki[1], Vladyslav Zbarskyy[2], Marvin Walter[2], Henning Schuhmann[1], Michael Seibt[1], and Markus Münzenberg[2] — [1]IV. Physikalisches Institut, Georg-August-Universität Göttingen, Germany — [2]I. Physikalisches Institut, Georg-August-Universität Göttingen, Germany

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

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

We thank the DFG for funding the research through SFB602.

DS 29.48 Wed 15:00 Poster A

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

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

DS 29.49 Wed 15:00 Poster A

Plasma treatment of polydimethylsiloxane thin films — •Vladimir Danilov, Jürgen Meichsner, and Hans-Erich Wagner — Institute of Physics, University of Greifswald, Felix-Hausdorff-Str. 6, 17487 Greifswald, Germany

Plasma modification of polydimethylsiloxane (PDMS) thin films was studied by means of Fourier-Transform-Infrared-Reflection-Absorption-Spectroscopy. The spin-coated PDMS films (10 nm - 100 nm) were prepared on aluminium coated glass substrates, and their thickness was measured by spectroscopic ellipsometry. The direct plasma treatment is compared with the plasma radiation, only, in argon and hydrogen rf plasmas, respectively. Evolution of IR spectra was monitored, and the changes of PDMS characteristic absorption bands (absorbance, broadening, shifting) as well as the formation of new bands are discussed. In particular, the appearance of new band at 1230 cm^{-1} was observed, and it was identified as LO phonon band of $\mathrm{SiO_x}$. For analysis of the Si-O-Si asymmetrical vibration band the deconvolution of this band was performed using Gaussian peaks.

DS 29.50 Wed 15:00 Poster A

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

Plasma polymerized ethylenediamine (PPEDA) thin films (15 - 80 nm) were deposited on different substrate materials (TiOx, Si, Al) in capacitively coupled radio frequency plasma. Beside the optimization of the plasma processing parameters, the plasma chemical conversion of the precursor ethylenediamine (EDA) was studied by means of the plasma induced optical emission spectroscopy, analysing the CN emission at 384 nm as well as the emission of H_α (656 nm) and Ar (750 nm). The FTIR (IRRAS) absorption spectra of deposited thin films reveal characteristic absorption of NH (3000 and 3500 cm^{-1}), CH (2900 cm^{-1}), CN/CC (2150 cm^{-1}), and NH_2 (1600 cm^{-1}). Comparing the thin film spectra with that of the liquid precursor EDA, the films are strongly cross linked. The refractive index shows normal dispersion in the visible spectral region, and in dependence on the deposition parameters anomal dispersion in the UV. The XPS analysis combined with derivatisation technique provides information about the NH_2 functional groups. Biomedical test substrates covered with PPEDA thin films show significant increase in cell adhesion. The investigations were realized within the BMBF collaborative research project "Campus PlasmaMed", grant no 13N9774.

DS 29.51 Wed 15:00 Poster A

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

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

DS 29.52 Wed 15:00 Poster A

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

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

DS 29.53 Wed 15:00 Poster A

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

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

DS 29.54 Wed 15:00 Poster A

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

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

DS 29.55 Wed 15:00 Poster A

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

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

DS 29.56 Wed 15:00 Poster A

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

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

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

DS 30: Invited Koopmans

Time: Thursday 9:30–10:15 Location: H2

Invited Talk DS 30.1 Thu 9:30 H2

Spin in organics, a new route to spintronics — •Bert Koopmans — Depertment of Applied Physics, Eindhoven University of Technology, Eindhoven, The Netherlands

Organic spintronics aims at new device functionality by combining the field of magneto- or spinelectronics with that of organic or plastic electronics. In hybrid organic spin-valves, an organic semiconducting film is sandwiched between two ferromagnetic thin films, aiming at magnetoresistive effects that exploit the long spin relaxation time of organic materials. Alternatively, organic magnetoresistance (OMAR) has been observed in devices without any ferromagnetic components, displaying up to 30% at room temperature, and at relatively small magnetic fields (5 mT). In this presentation, I will introduce this novel OMAR effect, and show that it provides us with entirely new physics, combining 'spin blocking' mechanisms with specific features of the behaviour of devices operating in bipolar space-charge limited current regime. Finally it will be shown that weak hyperfine fields from the hydrogen atoms in the organic materials are crucial for a proper understanding of both OMAR and organic spin valves.

DS 31: Molecular Spintronics - Current Status and Challenges I (Focused Session)

Time: Thursday 10:30–12:45 Location: H2

Topical Talk DS 31.1 Thu 10:30 H2

Spintronics with Organic Semiconductors — •V. Alek Dediu — ISMN-CNR, Via Gobetti 101, 40129 Bologna

Spin electronics, in its aim to compete with conventional electronics, is always looking for new and more performing materials. Conjugated organic semiconductors represent a possible breakthrough in the discipline, due to their weak spin-orbit scattering and their chemical flexibility. The former produces extremely long spin flip times, enabling spin manipulation processes in various devices. The latter promises an enormous choice of materials. Here I propose an outlook of the main issues in the field of organic spintronics as well as I present most recent results from our laboratory on magnetic and multifunctional effects in hybrid organic-inorganic devices. Finally, I will discuss the challenges in the field and possible strategies to outcome them.

Topical Talk DS 31.2 Thu 11:00 H2

Muon measurements of spin transport and dynamics in organic semiconductors — •Alan Drew — Physics Department, Queen Mary University of London, UK

Organic semiconductors fall into a class of materials that shows significant potential for future applications and as a result, the field is becoming extremely topical. However, there is a lack of suitable techniques that can yield information on intrinsic spin and charge carrier dynamics in organic materials.

Low Energy Muon Spin Rotation can directly measure the depth resolved spin polarisation of charge carriers in organic spin injection devices [1]. Using this technique, it is possible to separate out the various contributions to spin decoherence, differentiating between interface and bulk spacer layer effects. I will present the first direct measurement of spin coherence length and initial polarisation of injected electrons in a realistic and fully functional organic spin valve. Bulk muon techniques can also be used to probe the charge carrier and spin dynamics of organic semiconductors on a molecular lengthscale [2]. I will present measurements of temperature dependent electron spin relaxation rates, on a series of organic molecules of different morphology and molecular structure, which points towards some generality of the underlying spin scattering mechanisms in organic materials [3].

[1] A. J. Drew et al., Nature Materials 8, 109 (2009) [2] A. J. Drew et al., Phys. Rev. Lett. 100, 116601 (2008) [3] L. Schulz et al., in preparation

DS 31.3 Thu 11:30 H2

Engineering of the energy level alignment at organic semiconductor interfaces by intra-molecular degrees of freedom: transition metal phthalocyanines — •Mandy Grobosch[1], Victor Y. Aristov[1,2], Olga V. Molodtsova[1], Christian Schmidt[1], Brian P. Doyle[3,4], Stefano Nannarone[3], and Martin Knupfer[1] — [1]IFW Dresden, D-01069 Dresden, Germany — [2]nstitute of Solid State Physics, Russian Academy of Sciences, Moscow, Russia — [3]University of Johannesburg, PO Box 524 Auckland Park — [4]TASC-INFM Laboratory Trieste, Italy

The fact, that the transition metal ion in the central cavity of the Pc's can have a magnetic moment is a characteristic feature of TMPc's, and therefore these phthalocyanines can also show fascinating magnetic properties. We have determined the energy level alignment at interfaces between various transition metal phthalocyanines and gold using photoemission spectroscopy. Our results demonstrate that the transition metal center has a strong influence on the electronic properties of the phthalocyanine films as well as their interfaces with gold. This offers a route to adjust the hole injection barrier via the choice of otherwise equivalent molecular organic semiconductors. In particular, the interfaces MnPc/Au and CoPc/Au are characterized by a small hole injection barrier, which would be advantageous for applications. These are directly related to the presence of metal 3d states closest to the chemical potential; a fact that is also reflected in smaller ionization potentials for MnPc and CoPc as compared to other phthalocyanines. For details see: M. Grobosch et al., J. Phys. Chem. C 113, 13219 (2009).

DS 31.4 Thu 11:45 H2

Magnetic transition metal phthalocyanine thin films: electronic properties via K doping — •Olga Molodtsova[1], Victor Aristov[1,2], Volodymyr Maslyuk[3], Denis Vyalikh[4], Alexei Preobrajenski[5], Ingrid Mertig[3], Thomas Bredow[6], and Martin Knupfer[1] — [1]IFW Dresden, Germany — [2]ISSP RAS, Russia — [3]Uni Halle, Germany — [4]TU Dresden, Germany — [5]Max-Lab Lund, Sweden — [6]Uni Bonn, Germany

Magnetic transition metal phthalocyanines (MTM-Pc's) are considered as materials for development of low dimensional molecular magnets and quantum computers. To make further progress in development such devices both the understanding and the tailoring of the physical, chemical and transport properties of the organic semiconductor components are required. Due to the exceptional ability to incorporate electron acceptors and/or donors into molecular crystals the control of their electronic properties is possible. In this work the evolution of electronic structure of the MTM-Pc's with potassium doping has been studied by means of photoemission spectroscopy, near-edge X-ray absorption fine structure and DFT calculations. The DFT calculations and detailed analysis of the core-level spectra permit us to suggest possible lattice sites for the potassium ions. The data disclosed filling of the lowest unoccupied molecular orbital upon doping and associated changes of the core level absorption spectra. None of the films prepared in our studies showed a finite electronic density of states at the Fermi level. Acknowledgements: This work was supported by the RFBR under grant no. 08-02-01170.

DS 31.5 Thu 12:00 H2

Magnetic transition metal phthalocyanine thin films on Au(001): ordering and electronic structure — •Victor Aristov[1,2], Volodymyr Maslyuk[3], Olga Molodtsova[1], Ingrid Mertig[3], Thomas Bredow[4], and Martin Knupfer[1] — [1]IFW Dresden, Germany — [2]ISSP RAS, Russia — [3]Uni Halle, Germany — [4]Uni Bonn, Germany

At the present time magnetic transition metal phthalocyanines (MTM - Pc's) are considered as objects for the elaboration of low dimensional molecular magnets because they are supposed as possible candidates for potential applications in high-density information storage and quantum computers. Such possible applications give a strong motivation to characterize and investigate the ordering and electronic properties of MTM-Pc thin films since this determines the performance of devices. In this presentation we report the results of investigations of the molecular ordering, as well as the core-levels, valence band and unoccupied electronic states of the organic semiconductors MTM-Pc in situ grown on Au(001) surface under UHV conditions. The studies were done using a combination of experimental and theoretical techniques, by means of quantum-chemical calculations at DFT level, direct and resonant photoemission and NEXAFS. The experimentally obtained electronic features are in a good agreement with ab initio density of state results allowing a detailed site specific insight into the system. Acknowledgments: This work was supported by the RFBR under grant no. 08-02-01170.

Topical Talk DS 31.6 Thu 12:15 H2

Role of the van der Waals interaction on the adsorption of organic molecules on surfaces — •Nicolae Atodiresei — Institut für Festkörperforschung, Forschungszentrum Jülich

The design of nanoscale molecular elements in multifunctional devices relies on a clear understanding of the physics at electrode-molecule interfaces with a particular emphasis on the functionality of specific molecules in a given organic-inorganic surface environment. Using *ab initio* simulations and appropriate methods to account for the long-range dispersion effects we have performed studies on several organic molecules adsorbed on non-magnetic and ferromagnetic surfaces. Our results show that the alignment of the molecular orbitals at adsorbate-substrate interface depends on the number of heteroatoms present in an aromatic ring and, as a direct consequence, for a flat adsorption geometry, the molecule-surface van der Waals interaction involves not only the π-like orbitals which are perpendicular to the molecular plane but also σ-like orbitals delocalized in the molecular plane. In the case of perpendicular adsorption geometries we demonstrate that the position of the heteroatoms in the aromatic rings can be used to precisely tune the HOMO-LUMO gap making possible a chemical identification of the specific molecular species embedded into a molecular layer. Furthermore, our calculations demonstrate that, for specific types of organic molecules, taking into account the non-local correlation effects responsible for the long range van der Waals interaction is essential to correctly describe the charge transfer at the interface which yields the formation of molecule-surface hybrid states.

DS 32: Invited Limot

Time: Thursday 14:00–14:45 Location: H2

Invited Talk DS 32.1 Thu 14:00 H2

Spintronics below one nanometer — •Laurent Limot — Institut de Physique et Chimie des Matériaux de Strasbourg, UMR 7504, Université de Strasbourg, France

Spintronics has seen a considerable effort aimed at improving the quality of devices because there is a growing awareness that structural details may substantially affect the magnetoresistive response. To learn more about these disruptive effects, one possibility consists in focusing on the interplay between structure-related and spin-related properties in model magnetic systems. As an example we will present recent SP-STM measurements of a single Co-Phthalocyanine molecule interacting with a magnetic surface. We will then show how to go one step further in order to engineer a spintronic device with the scanning tunneling microscope. As will be exemplified for a Kondo atom, this consists in suppressing the vacuum barrier by bringing the tip of the microscope into contact with well-characterized individual atoms and molecules.

DS 33: Molecular Spintronics - Current Status and Challenges II (Focused Session)

Time: Thursday 15:00–16:00 Location: H2

Topical Talk DS 33.1 Thu 15:00 H2

Spin-dependent tunneling through a single molecule with intramolecular resolution — •Roland Wiesendanger — Institut für Angewandte Physik und Interdisziplinäres Nanowissenschafts-Centrum Hamburg, Universität Hamburg, D-20355 Hamburg, wiesendanger@physnet.uni-hamburg.de, www.nanoscience.de

Molecular spintronics based on the injection, transport, and detection of spin currents through a single magnetic molecule opens up fascinating perspectives for future nanoscale storage or logic devices. Progress in this exciting field of research depends on a detailed characterization of the electrode-molecule interface at high spatial resolution. We have applied spin-polarized scanning tunneling microscopy (SP-STM) and spectroscopy (SP-STS) [1] to study the energy- and spin-dependent tunneling through individual phthalocyanine molecules as function of their orientation with respect to the substrate lattice and as function of the magnetization states of substrate and SP-STM tip. Interestingly, a strong spin-dependent intramolecular contrast is observed related with a significant difference in spin-dependent current flow through the central metal ion and the surrounding ligands. Our experimental results are in good agreement with first-principles calculations including the van-der Waals interaction between molecule and substrate.

[1] R. Wiesendanger, Rev. Mod. Phys. 81, 1495 (2009).

Topical Talk DS 33.2 Thu 15:30 H2

Tunneling through magnetic molecules: what can we learn from the master equation? — •Carsten Timm[1], Florian Elste[2], and Binhe Wu[3] — [1]Technische Universität Dresden, Germany — [2]Columbia University, New York, USA — [3]Max-Planck-Institut für Physik komplexer Systeme, Dresden, Germany

Progress in molecular spintronics requires an improved understanding of electronic transport through magnetic molecules far from the linear-response regime. For weak hybridization with the electronic leads, the method of choice for the theoretical description is the master equation. A number of effects relevant for spintronics, such as spin blockade and spin amplification, will be reviewed. The master equation also sheds light on the spin *dynamics*, as will be illustrated by the examples of spin relaxation and the current-noise spectrum.

DS 34: Invited Weightman

Time: Thursday 16:15–17:00 Location: H2

Invited Talk DS 34.1 Thu 16:15 H2

Probing the structure and dynamics of biomolecules adsorbed on surfaces. — •Peter Weightman — Physics Department, University of Liverpool, Oxford Street, Liverpool, L69 3BX UK

This talk will begin with a review of the contribution that Reflection Anisotropy Spectroscopy (RAS) [1] can make to the study of molecules adsorbed on surfaces. The technique can be used to determine the three dimensional orientation of a molecule adsorbed at a metal-liquid interface [2], to monitor conformational change in proteins and interactions between adsorbed molecules in real time [3,4] and to probe mechanisms of DNA hybridisation [5].

An account will also be given of the potential of research with free electron lasers and terahertz techniques to provide insight into mechanisms of biological organisation important in photosynthesis.

[1] P. Weightman, D.S. Martin, R.J. Cole and T. Farrell, Rep. Prog. Phys. 68 1251 (2005) [2] P. Weightman, G.J. Dolan, C.I. Smith, M.C. Cuquerella, N.J. Almond, T. Farrell, D.G. Fernig, C. Edwards and D.S. Martin, Phys. Rev. Lett. 96 86102 (2006) [3] H.L. Messiha, C.I. Smith, N.S. Scrutton and P. Weightman, Euro. Phys. Lett. 83 18004 -1 (2008) [4] R.LeParc, C.I. Smith, M.C. Cuquerella, R.L. Williams, D.G. Fernig, C. Edwards, D.S. Martin and P. Weightman, Langmuir 22 3413 (2006) [5] C.I. Smith, A. Bowfield, M.C. Cuquerella, C.P. Mansley, T. Farrell, P. Harrison, D.S. Martin, D.G. Fernig, C. Edwards, J.E. Butler, R.J. Hammers, B. Sun, X. Wang and P. Weightman, Euro. Phys. Lett. 85 18006 (2009)

DS 35: Biomolecular and Functional Organic Layers I (Focused Session)

Time: Thursday 17:15–19:00 Location: H2

Topical Talk DS 35.1 Thu 17:15 H2

Surface enhanced infrared spectroscopy - pushing the detection limit towards zeptomolar sensitivity — •Frank Neubrech, Daniel Weber, Jörg Bochterle, and Annemarie Pucci — Kirchhoff - Institut für Physik, Universität Heidelberg

Surface enhanced infrared absorption (SEIRA) of molecules on metal films is known for many years but is still suffering from too small enhancement factors. Similar to surface enhanced Raman scattering, the electromagnetic field enhancement gives the main contribution to SEIRA signals. For adsorbates on metal nanoparticle-films average enhancement factors of more than three orders of magnitude were obtained. If metal nanoantennas are involved, the magnitude of the near-field amplitude at the fundamental (and also higher order) plasmon resonance reaches some ten times the external field value and therefore lowers the detection limit significantly. To analyse this kind of SEIRA quantitatively, well-defined monolayers of octadecanethiol on nanoantennas were investigated by means of infrared micro-spectroscopy. For individual nanoantennas, we have proven extraordinary enhancement factors up to 500 000 (ratio between enhanced infrared signal size and infrared absorption of the same number of molecules). The enhanced vibration signals show Fano-type line shapes due to dipolar coupling between molecular and plasmonic excitations.[1] Further increase of enhancement factors via near-field confinement in nanogaps of resonant nanoantenna arrays is under investigation.[2]

[1] F. Neubrech *et al*, Phys. Rev. Lett. 101, 157403, 2008.
[2] A. Pucci *et al*, submitted to Phys. Stat. Sol (B) 2009.

DS 35.2 Thu 17:45 H2

Optical Characterization of Cytosine Thin Films — •Dana M. Rosu, Simona Pop, Norbert Esser, and Karsten Hinrichs — ISAS - Institute for Analytical Sciences, Department Berlin, Albert-Einstein-Str. 9, 12489 Berlin, Germany

Due to their application in the fabrication of biomolecular electronic devices, the cytosine thin films are of high technological interest. Therefore, the understanding of the optical and structural properties of these films is important for the controlled design of cytosine thin films. In the present work, results of a complex study on thin films of cytosine on Si with a thickness between 10 nm and 125 nm are presented. The thin films were obtained by evaporation in high vacuum and investigated using different optical techniques. Thickness and dielectric function of the cytosine films were determined from VIS ellipsometric measurements while molecular orientation was studied by IR ellipsometry and reflectance anisotropy spectroscopy (RAS). Different organization of the molecules on the substrate is observed for different film thicknesses. The IR mapping ellipsometer [1], located at the BESSY II synchrotron facility was used in order to study the structural and thickness homogeneity of the samples.

References: [1]Gensch M., Esser N., Korte E. H., Schade U., Hinrichs K. Infrared Physics and Technology 2006, 49, 74

DS 35.3 Thu 18:00 H2

IR Spectroscopic Characterization of Carboxyl Acid-terminated Au Surfaces: Towards Biosensors — •Guoguang

Sun[1], Marc Hovestädt[2], Xin Zhang[3], Dana Maria Rosu[1], Bernhard Ay[2], Rudolf Volkmer[2], Jörg Rappich[3], and Karsten Hinrichs[1] — [1]ISAS- Institute for Analytical Sciences, Department Berlin, Albert-Einstein-Str. 9, 12489 Berlin, Germany — [2]Charité Universitätsmedizin Berlin, Institut für Medizinische Immunologie, Abteilung Molekulare Bibliotheken, Hessische Str. 3-4 , 10115 Berlin, Germany — [3]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Insitut für Silizium-Photovoltaik, Kekuléstr. 5, 12489 Berlin, Germany

Specific vibrational bands (C=O, amide I and amide II) were used for interpretation of IR spectra of the thin films ($d<10$ nm) achieved in every preparation step. The molecular interactions between the functional groups on the surface and the selected peptide as well as anti-glutathione S-transferase (GST) antibody were proved by IR ellipsometry spectra. The characteristic IR-spectra after antibody adsorption suggest that an IR-based biosensor could probably be built for an application.

DS 35.4 Thu 18:15 H2

Optical Properties of Thin Films of ZnTPP oligomers — •Simona Pop[1], Mathias Senge[2], Oliver Locos[2], Karsten Hinrichs[1], Xin Zhang[3], Jörg Rappich[3], Christoph Cobet[1], and Norbert Esser[1] — [1]ISAS-Institute for Analytical Sciences, Albert-Einstein-Str.9, D-12489 Berlin, Germany — [2]School of Chemistry, SFI Tetrapyrrole Laboratory, Trinity College Dublin, Dublin 2, Ireland — [3]Helmholtz-Zentrum Berlin for Materials and Energy GmbH, Institute for Silicon Photovoltaics, Kekuléstrasse 5, D-12489 Berlin, Germany

Porphyrin oligomers are of great interest for technological applications such as biosensors, solar cells and OFETs (organic field-effect transistors). These materials exhibit extraordinary optical and electronic properties due to the π-conjugation. The main characteristics of these oligomers as a consequence of π-conjugation are the high polarisabilities and low energy electronic transitions. Here, thin films of ZnTPP (zinc tetraphenylporphyrin) monomer and dimer were investigated by means of spectroscopic ellipsometry. In the case of the π-conjugated ZnTPP dimer, the porphyrin units are connected through an ethylene bridge. The films were prepared by means of spin-coating method on silicon substrates. The dielectric functions of ZnTPP monomer and dimer are derived from ellipsometrical measurements by employing a three-phase optical model. As expected, the ZnTPP dimer films exhibit a strong red-shift of the first absorption structure, namely Q-band, compared to the monomer case. The spectral changes observed for the ZnTPP dimer films can be interpreted in terms of strong electronic interactions and weak electrostatic ones.

Topical Talk DS 35.5 Thu 18:30 H2

Infrared spectroscopic ellipsometry for the in-situ investigation of responsive polymer brushes — •Dennis Aulich[1], Eva Bittrich[2], Klaus-Jochen Eichhorn[2], Petra Uhlmann[2], Manfred Stamm[2], Martin Brücher[3], Roland Hergenröder[3], Olha Hoy[4], Igor Luzinov[4], Norbert Esser[1], and Karsten Hinrichs[1] — [1]Leibniz-Institut für Analytische Wissenschaften - ISAS - e.V., Albert-Einstein-Str. 9, 12489 Berlin — [2]Leibniz-Institut für Polymerforschung Dresden e.V., Hohe Str. 6, 01069 Dresden — [3]Leibniz-Institut für Analytische Wissenschaften - ISAS - e.V., Otto-Hahn-Str. 6b, 44227 Dortmund — [4]School of Materials Science and Engineering, Clemson University, Clemson, SC 29634-0971, USA

Responsive polymer brushes offer a wide range of applications. Due to the possibility of changing the surface properties by external stimuli such as pH, solvent, temperature or electric field, mixed polymer brushes can control protein adsorption, wettability or adhesion of a surface. In order to understand the complex behavior of this surface functionalization, the single mechanisms like switching of polymer brushes and the adsorption of protein layers have to be well investigated. Infrared Spectroscopic Ellipsometry (IRSE) is a suitable method for in-situ measurements of polymer brush systems in solution and gives direct insight into the response of the brush to external stimuli by observation of the dissociation of charged groups in the polymer material. Various brush systems were investigated with in-situ IRSE and compared with additional methods such as VIS-ellipsometry, x-ray standing waves and contact angle measurements.

DS 36: Thin Film Characterisation: Structure Analyse and Composition (XRD, TEM, XPS, SIMS, RBS, ...) I

Time: Thursday 9:30–11:00 Location: H8

DS 36.1 Thu 9:30 H8

GD OES analysis of thin film samples with application of pulsed discharge. — •Varvara Efimova[1], Volker Hoffmann[1], and Jürgen Eckert[1,2] — [1]IFW Dresden, Institut für Komplexe Materialen, Helmholtzstraße 20, 01069 Dresden, Germany — [2]TU Dresden, Institut für Werkstoffwissenschaft, D-01062, Dresden, Germany

The application of a pulsed power supply of glow discharge (GD) in optical emission spectrometry (OES) has a number of advantages in comparison with the continuous one [1]. Because of the slower sputtering and less heating of the sample, pulsed discharge is preferable for the analysis of thin layers and heat-sensitive samples.

However, the use of pulsed GD (PGD) in commercial spectrometers has still some limitations. Firstly, the influence of PGD parameters on the analytical performance is not yet enough investigated. Secondly, it is difficult to quantify the profiles measured with PGD, because the existing quantification model is established for the continuous discharge.

In the present work the methodic of the optimization of PGD parameters has been developed. According to the studies carried out, the measurement of depth profiles of thermally fragile and thin layered samples with pulsed radio frequency GD OES has been optimized. To some of the measured depth profiles a quantification procedure has been applied. The results of the quantification have shown that the existing quantification model is valid also for the pulsed discharge, if the measurement is performed under the same conditions as the calibration.

[1] W.W. Harrison, J. Anal. At. Spectrom., 13, 1051 (1998).

DS 36.2 Thu 9:45 H8

Structural investigations of the grain growth induced by focused-ion-beam irradiation in thin magnetic films — •Olga Roshchupkina, Jörg Grenzer, Monika Fritzsche, and Jürgen Fassbender — Institute of Ion Beam Physics and Materials Research, Forschungszentrum Dresden-Rossendorf, P. O. Box 51 01 19, 01314 Dresden, Germany

Focused ion beam (FIB) techniques are one way to modify locally the properties of magnetic thin films. In previous works it was demonstrated that focused-ion-beam irradiation causes a considerable grain growth in magnetic thin films under certain conditions and therefore a change of their magnetic properties [1]. Although the grain growth can be already qualified by simple REM images a crystallographic tool is needed for a qualitative analysis. We used the advantage of non-destructive X-ray diffraction to study the grain growth.
A magnetic thin film of $50nm$ thick permalloy film ($\mathrm{Fe}_{0.2}\mathrm{Ni}_{0.8}$) sputtered on Si was used for the investigations. We have analyzed two simple parameters such as the grain size and the microstrain depending on the ion dose and beam current. Due to the very small structures created by focused-ion-beam techniques (usually less then $0.4x0.4mm^2$ size) an optimized X-ray laboratory setup with a focused X-ray beam of $200\mu m$ was used.

[1] C.M. Park and J.A. Bain, J. Appl. Phys. 91, 6830(2002).

DS 36.3 Thu 10:00 H8

Surface characterization after subaperture Reactive Ion Beam Etching — •André Miessler, Thomas Arnold, and Bernd Rauschenbach — Leibniz-Institut für Oberflächenmodifizierung (IOM), Permoserstrasse 15, D-04318Leipzig, Germany

In usual ion beam etching processes using inert gas (Ar, Xe, Kr...) the material removal is determined by physical sputtering effects on the surface. The admixture of suitable gases ($CF_4 + O_2$) into the glow discharge of the ion beam source leads to the generation of reactive particles, which are accelerated towards the substrate where they enhance the sputtering process by formation of volatile chemical reaction products.

During the last two decades research in Reactive Ion Beam Etching

(RIBE) has been done using a broad beam ion source which allows the treatment of smaller samples (diameter sample < diameter beam). Our goal was to apply a sub-aperture Kaufman-type ion source in combination with an applicative movement of the sample with respect to the source, which enables us to etch areas larger than the typical lateral dimensions of the ion beam. Concerning this matter, the etching behavior in the beam periphery plays a decisive role and has to be investigated. We use interferometry to characterize the final surface topography and XPS measurements to analyze the chemical composition of the samples after RIBE.

DS 36.4 Thu 10:15 H8

RBS and resonant scattering analysis of thin oxidic films prepared by sputtering — •Dieter Mergel[1], Hans-Werner Becker[2], and Detlef Rogalla[2] — [1]Universität Duisburg-Essen, FB Physik, 47048 Duisburg — [2]Ruhr-Universität Bochum, Dynamitron Tandem Labor des RUBION, 44780 Bochum

The oxygen content in various oxidic thin films has been determined from alpha scattering spectra based upon gauging with a rutile and a $SrTiO_3$ crystal. Both RBS and scattering with the 3.04 MeV resonance (for O) were applied and compared to each other.

Main findings are:

- Gradient in O-content of TiO_2 prepared by reactive magnetron sputtering at 300°C at various oxygen partial pressures.
- Oxygen surplus in ITO films prepared by rf-diode sputtering.
- Variation in the oxygen content of nominal Cr_2MnO_4 prepared by magnetron sputtering at 350°C to 650°C.

DS 36.5 Thu 10:30 H8

A New High-Resolution Scanning Electron Microscope for the in-situ investigation of ion beam modifications of solid surfaces — •Wolfgang Bolse[1], Sankarakumar Amirthapnadian[1,2], and Florian Schuchart[1] — [1]Institut für Halbleiteroptik und Funkitonelle Grenzflächen, Universität Stuttgart — [2]on leave from: IGCAR, Kalpakkam, India

A High Resolution Scanning Electron Microscope (HRSEM), which allows for in-situ investigation of swift heavy ion (SHI) induced modifications of solid surfaces with nm resolution, has been installed at the M-branch of the UNILAC ion accelerator at GSI in Darmstadt. The HRSEM is a standard SUPRA-40 SEM by CARL ZEISS SMT with an annular in-lens secondary electron detector, an Everhart-Thornley scintillation detector and a retractable 4-quadrant Si-diode with a hole in the center. Two ports of the microscope chamber have been modified such that it could be integrated into the UNILAC beam line and the ion beam can pass through the focal zone of the upright electron lens. In addition to the standard eucentric stage, a special stage was designed which allows to continuously vary the tilt angle of the sample from normal incidence of the electron beam to normal incidence of the ion beam, as well as for continuous azimuthal rotation of the sample. In this report we will introduce the setup and discuss why in-situ investigation of structure formation under SHI bombardment outmatches conventional ex-situ experiments. We will demonstrate the potential of the instrument by presenting the results of our first in-situ experiments on SHI induced dewetting of thin oxide films.

DS 36.6 Thu 10:45 H8

Structure of Co/Pt multilayers on gold particle arrays — •Herbert Schletter[1], Carsten Schulze[1], Denys Makarov[1], Alan Craven[2], Sam McFadzean[2], Manfred Albrecht[1], and Michael Hietschold[1] — [1]Institute of Physics, Chemnitz University of Technology, 09107 Chemnitz — [2]Department of Physics and Astronomy, University of Glasgow, Glasgow G12 8QQ, Scotland, UK

Nanostructuring of thin films is used in a variety of applications and attracts scientific as well as technological interest. One way to realize such structuring is by using particle arrays as templates onto which the films are deposited [1]. In the present study, gold particles with diameters of 20 nm to 60 nm are used to implement this concept. A 17 nm thick Co/Pt multilayer film with out-of-plane magnetic anisotropy was deposited onto these particles. Besides magnetic characterisation, a detailed structural investigation is essential for the understanding of magnetic properties. In this regard, SEM was used to analyze the particle assembly as well as the surface morphology of the film. Further details about the magnetic films were gathered with cross sectional TEM and EELS Spectrum Imaging. It was found, that for 60 nm and 40 nm particles, the magnetic layer forms a closed film which follows the morphology of the particle arrangement. In contrast to that, on 20 nm particles the roughness of the magnetic film is of the same size as the height variations induced by the particles. These findings allowed conclusions about magnetic coupling behaviour and served to clarify differences found in the magnetization reversal process.

[1] M. Albrecht et al., Nature Materials 4 (2005) 203.

DS 37: Thin Film Characterisation: Structure Analyse and Composition (XRD, TEM, XPS, SIMS, RBS, ...) II

Time: Thursday 11:15–12:45 Location: H8

DS 37.1 Thu 11:15 H8

Rare-Earth-Oxide Ultrathin Films — •Maraike Ahlf[1], Marvin Zöllner[1], Mareike Ahlers[2], Mathias Wickleder[2], and Katharina Al-Shamery[1] — [1]University of Oldenburg, Physical Chemistry 1 — [2]University of Oldenburg, Inorganic Chemistry, Germany

Increasing speed of development in microelectronics as well as in catalysis leads to the need of high performance thinfilm materials e.g. as gate-oxides in MOSFETs, new OLED applications or thinfilm coatings on catalysts. Especially in semiconductor industries the miniaturization of the microelectronic components requires new materials having higher dielectric constants and larger band gaps than conventionally used SiO_2 as gate-oxide to avoid quantummechanical tunneling with concomitant high leakage and high heat diffusion rates. Conventionally used methods for thinfilm deposition (e.g. PVD, CVD) suffer from problems such as carbon impurities within the deposited layers and formation of interfacial layers. Rare-earth oxides are potential candidates to replace SiO_2 as gate-oxide due to their electrical properties. Alternatively they are good candidates for OLED applications due to their luminescence. A radically new approach using new rare-earth based inorganic designer precursors which may easily be realized and incorporated into device production will be presented. In and ex UHV-Experiments have been done to study the constitution of the thin films, the crystallization process and the decomposition mechanism of the precursors on the surface using XPS, STM, AFM, SEM, TPD, TGA and TEM analyses. The precursors are expected to decompose carbonfree to form the oxide and gaseous decomposition products.

DS 37.2 Thu 11:30 H8

GIXRF in the soft X-Ray range used for the characterization of ultra shallow junctions — •Burkhard Beckhoff[1], Philipp Hönicke[1], Damiano Giubertoni[2], and Giancarlo Pepponi[2] — [1]Physikalisch-Technische Bundesanstalt, Abbestr. 2-12, 10587 Berlin, Germany — [2]Fondazione Bruno Kessler, via Sommarive 18, 38100 Povo, Trento, Italy

Grazing Incidence X-Ray Fluorescence (GIXRF) analysis in the soft X-ray range provides excellent conditions for exciting B-K and As-$L_{iii,ii}$ shells. The X-ray Standing Wave field (XSW) associated with GIXRF on flat samples is used as a tunable depth sensor to gain information about the implantation profile. This technique is very sensitive to near surface layers. It is therefore well suited for the study of ultra shallow dopant distributions. Arsenic implanted (implantation energies between 0.5 keV and 5.0 keV) and Boron implanted (implantation energies between 0.2 keV and 3.0 keV) Si wafers have been used to compare SIMS analysis with GIXRF analysis.

The measurements have been carried out at the electron storage ring BESSY II using monochromatized undulator radiation of well-known radiant power and spectral purity. The use of an absolutely calibrated energy-dispersive detector for the registration of the B-Kα and As-Lα fluorescence radiation allows for the absolute determination of the retained dose. An estimate of the concentration profile has been obtained by fitting the measurements with profiles derived by simulation of the implantation process. A good match among the total retained dose measured with the different techniques has been observed.

DS 37.3 Thu 11:45 H8

Advanced species depth-profiling with a photon-in photon-out method — •Beatrix Pollakowski and Burkhard Beckhoff — Physikalisch-Technische Bundesanstalt, Abbestr. 2-12, 10587 Berlin

Characterizing multi-layered systems with layer thicknesses of up to 10 nm, which is beyond conventional electron information depths and sensitivity, only spectroscopic method based on photon excitation and detection may provide information without any destructive modifications of the specimens. The presented photon-in photon-out method GIXRF-NEXAFS [1] allows for a non-destructive analysis with respect to the chemical bonds of deeply buried single layers. Considering the investigation of buried interfaces or gradient layers this approach may gain in importance as alternative method. The intensity of the X-ray standing wave (XSW) field determining GIXRF characteristics is utilized as a tunable marker to keep the mean penetration depth constant in the respective layer of interest.

The multi-layered systems investigated consist of a titanium oxide and metallic titanium layer, separated from each other by a 2 nm C layer. For the respective experiment, well-characterized monochromatic synchrotron radiation of the electron storage ring BESSY II and absolutely calibrated instrumentation was employed. GIXRF-NEXAFS measurements at the Ti-$L_{iii,ii}$ absorption edges with angular correction based upon prior XSW simulation demonstrate the high potential of the approach for analyzing novel materials and may provide access to buried interfaces by a differential approach.

[1] B. Pollakowski et al., Phys. Rev. B **77**, 235408 (2008)

DS 37.4 Thu 12:00 H8

Oberflächenanalyse von hocheffizienten Cu(In,Ga)Se_2 Solarzellenabsorberschichten — •J. Lehmann, S. Lehmann, S. Sadewasser, C.A. Kaufmann, T. Rissom, R. Caballero, A. Grimm, I. Lauermann und M.Ch. Lux-Steiner — Helmholtz-Zentrum Berlin für Materialien und Energie, Deutschland

Dünnschichtsolarzellen, basierend auf polykristallinen p-Typ Cu(In,Ga)Se_2 (CIGSe) Absorbern, weisen besonders hohe Wirkungsgrade (20%) auf. Durch intensive oberflächensensitive Charakterisierung wird gegenwärtig versucht, ein besseres Verständnis über Grenzflächen (z.B. Oberflächen, Korngrenzen) in diesen Solarzellen zu gewinnen. Verunreinigungen und Oxidation können dabei jedoch die Messergebnisse stark beeinflussen und teilweise verfälschen. Daher ist es wichtig, reproduzierbare und bezüglich Komposition und Kontamination definierte Oberflächen herstellen zu können. Hierzu wurden polykristalline CIGSe-Schichten definiert oxidiert und anschließend in basischen Lösungen (KCN bzw. NH_3) nasschemisch behandelt. Die Stöchiometrie sowie der Grad der Oxidation wurden mit Hilfe der Photoelektronenspektroskopie (XPS sowie UPS) oberflächensensitiv analysiert. Es zeigt sich, dass aufgrund der unterschiedlichen Affinitäten der Elemente zur Oxidation, die Oberflächenstöchiometrie der Probe verändert wird. Weiterhin konnte gezeigt werden, dass die Oberflächenbehandlung mit KCN in Bezug auf die Beseitigung der Oxide effektiver ist, als die Behandlung in ammoniakalischer Lösung. Die KCN-behandelte Oberfläche ist in seiner chemischen Struktur einer nicht an Sauerstoff ausgesetzten Oberfläche nahezu identisch.

DS 37.5 Thu 12:15 H8

Kationenordnung in $LaSrCoO_{3-x}$ Schichten auf $SrTiO_3$ — •Wolfgang Donner[1], Allan Jacobson[2] und Chonglin Chen[3] — [1]TU Darmstadt, Materialwissenschaften — [2]University of Houston, Chemistry — [3]University of Texas at San Antonio, Physics

Wir berichten über Synchrotronmessungen an dünnen epitaktischen $LaSrCo_{3-x}$ Schichten auf $SrTiO_3$. In Schichten, die *in situ* bei 400 Grad Celsius im Vakuum untersucht wurden, finden wir eine extrem grosse Ausdehnung (5.7%) in senkrechter Richtung gegenüber dem Zustand bei Normalbedingungen. Diese Ausdehnung wird durch die Ausbildung geordneter Sauerstoffleerstellen in Ebenen parallel zur Oberfläche verursacht. Wir finden dass diese Sauerstoffleerstellenordnung von einer Ordnung der La und Sr Kationen auf den A-Plätzen der Perowskitstruktur begleitet wird. Diese Kationenordnung tritt im Volumenmaterial nicht auf und ist durch die epitaktische Spannung verursacht.

DS 37.6 Thu 12:30 H8

Coincident Doppler Broadening measurement on embedded thin layers of different materials with a positron beam of variable energy — •Philip Pikart[1,2], Christoph Hugenschmidt[1,2], and Klaus Schreckenbach[1,2] — [1]ZWE FRM II, Lichtenbergstraße 1, 85747 Garching — [2]Technische Universität München, Physik Department E21, James-Franck Straße, 85748 Garching

Coincident Doppler Broadening (CDB) is particularly suited to study thin layers in a non-destructive way. Further, CDB is outstanding in its sensitivity to defects and precipitates, because the positron is used as a "nanoprobe". It diffuses thermally inside the sample, can be localized at a defect and then annihilates with an electron by the emission of gamma-radiation. The shape of the annihilation line is characteristic for chemical elements and defect types. Defects have a highly attractive potential for the diffusing positron, which leads to trapping in open volume defects. But also the trapping at precipitates and small clusters of a different material is possible. The aim of the presented experiment is to study the trapping at interfaces and thin layers. For this purpose, samples consisting of aluminum are grown with an embedded layer of gold, copper and chrome. These materials cover a wide range of positron affinities, so the trapping probability of a positron at the layer depends on the material and the layer thickness. CDBS-results of these samples are presented and explained by a one-dimension potential well model.

DS 38: Layer Properties: Electrical, Optical and Mechanical Properties

Time: Thursday 14:00–16:45 Location: H8

DS 38.1 Thu 14:00 H8

Modification of coherent acoustic phonon lifetimes in thin gold films by self-assembled monolayers — •Mike Hettich[1], Axel Bruchhausen[1], Oliver Ristow[1], Daniel Issenmann[1], Tobias Geldhauser[1], Ingo Wenke[2], Jürg Bryner[2], Jürg Dual[2], and Thomas Dekorsy[1] — [1]Department of Physics and Center of Applied Photonics, Universität Konstanz, Germany. — [2]Institute for Mechanical Systems, ETH Zürich, Switzerland.

The damping of coherent acoustic phonons in thin gold films has been investigated by asynchronous optical sampling (ASOPS)[1].

In order to measure the damping constants for various frequencies gold films are grown in a wedge shape. Different film thicknesses correspond to changes in the phonon oscillation frequencies which can therefore be measured by scanning over the sample surface.

For lower frequency phonons in the range of 50 GHz to ∼ 75 GHz a significant change in damping times is observed when a self assembled monolayer is added between the gold film and the substrate. The damping behaviour with and without self-assembled monolayer has been modelled with good agreement by a visco-elastic simulation.

[1] A. Bartels et al., Rev. Sci. Instr. 78, 035107 (2007).

DS 38.2 Thu 14:15 H8

Preparation and optical properties of metal–insulator–metal devices based on Ti and Ta for Photocurrent and Chemocurrent applications — •Kevin Stella[1], Domocos Kovacs[1], Detlef Diesing[1], Wolfgang Brezna[2], and Jürgen Smoliner[2] — [1]Institut für Physikalische Chemie, Universität Duisburg Essen — [2]Institut für Festkörperelektronik, Technische Universität Wien

The optical and electrical properties of amorphous titanium and tantalum oxide films with thicknesses of 2.5-5 nm are investigated. As characterisation methods we used experiments with bias and photoinduced currents in the respective metal-metal oxide-gold junctions. The photoyield recorded for wavelengths between 200 and 1600 nm shows significant increases for higher energies than 3.5 eV and 4.4 eV for the titanium respectively tantalum samples. These values coincide with the band gaps found in literature for bulk samples of the oxides. Deviations from the ideal behaviour can be observed in bias induced currents. Voltage pulse experiments and the subsequent recording of the current transient let us assign a trap density of several $10^{15} cm^{-2}$. Since the photoyield with energies below 2 eV shows a broadband like behaviour, one can discuss the role of the traps as midgap states in the oxide film. The bias dependence of the photocurrent is explained within a two flux model of photoelectrons and photoholes.

DS 38.3 Thu 14:30 H8

Preparation of polymer/metal-multilayers by pulsed laser deposition — •Susanne Seyffarth, Britta Lena Fuchs, Sarah Hoffmann, Inga Knorr, Cynthia Volkert, and Hans-Ulrich Krebs — Institut für Materialphysik, Universität Göttingen, Friedrich-Hund-Platz 1, D-37077 Göttingen

Polymer/metal multilayer structures are model systems to study the mechanical behaviours of composite materials. Layered polymer/metal nanocomposites consisting of poly(methyl methacrylate) PMMA and Cu were deposited by pulsed laser deposition (PLD) at room temperature. At this, a laser fluence of 120 mJ/cm^2 close to the deposition threshold was used to obtain smooth PMMA films without droplets, while for Cu a much higher laser fluence of 6 J/cm^2 is necessary. On the smooth polymer layers, the metal shows Volmer-Weber island growth leading for thin Cu-films to layered PMMA/Cu nanostructures with spherical metallic particles. For larger metal layer thicknesses, the metal layers are closed and PMMA/Cu multilayers are formed. The composition of PMMA was studied by infrared spectroscopy (FTIR). Atomic force microscopy (AFM) was used to study the surface morphology. Cross-section slices of the layered structures cut by focused ion beam (FIB) were examined by electron microscopy (SEM, TEM). It was found that indeed well layered PMMA/Cu-structures can be formed by PLD, but stress formation leads to buckles and waves of the metal layers as long as the PMMA layers are soft. In this contribution it is discussed how smooth metal and polymer layers can be obtained.

DS 38.4 Thu 14:45 H8

Investigation of structural and mechanical properties of pulsed laser deposited PMMA films — •Felix Schlenkrich[1], Britta Lena Fuchs[1], Peter Grossmann[2], Klaus Mann[2], and Hans-Ulrich Krebs[1] — [1]Institut für Materialphysik, Universität Göttingen, Friedrich-Hund-Platz 1, D-37077 Göttingen — [2]Laser-Laboratorium Göttingen e.V., Hans-Adolf-Krebs-Weg 1, D-37077 Göttingen

Smooth poly(methyl methacrylate) (PMMA) films without any droplets were pulsed laser deposited at a wavelength of 248 nm and a laser fluence of 125 mJ cm^{-2}. After deposition at room temperature the films obey a low universal hardness of only 3 N mm^{-2}. Thermal treatments up to 200°C, either during deposition or afterwards lead to a film hardening up to values of 200 N mm^{-2}.

Using a combination of complementary methods, two main mechanisms could be made responsible for this temperature induced hardening effect well above the glass transition temperature of 200°C. The first process is induced by the evaporation of chain fragments and low molecular mass material, which are present in the film due to the deposition process, leading to an increase of the average molecular mass and thus to hardening. The second mechanism can be seen in the cross-linking of the polymer film as soon as chain scission occurs at higher temperatures and the mobility and reactivity of the polymer material is high enough.

DS 38.5 Thu 15:00 H8

Photo-switchable azomolecule containing nanocomposites — •Christina Pakula[1], Christian Hanisch[1], Thomas Strunskus[1], Dordaneh Zargarani[2], Vladimir Zaporojtchenko[1], Rainer Herges[2], and Franz Faupel[1] — [1]Materialverbunde, Institut für Materialwissenschaft, CAU Kiel, Kaiserstr. 2, 24143 Kiel — [2]Otto Diels-Institut, CAU Kiel, Otto-Hahn-Platz 3/4, 24118 Kiel

We report on the electro-optical properties of nanocomposites based on polymer thin films with dissolved azobenzene chromophores containing embedded gold nanoparticles. The physical properties of these composites can be changed reversibly by illumination with UV and visible light, due to the conformational change of the switchable azomolecules. We examined the isomerization and the time dependence in optical switching with UV and visible light of an azobenzene ether dissolved in a PMMA (and a PDMS) matrix in combination with 2D and 3D gold nanoparticle arrays. The chromophore/polymer film was prepared by spin-coating and the metal clusters were deposited either by thermal evaporation or via sputtering and subsequently embedded into the polymer matrix. We discuss the photo-switchable changes in resistance of the 2D/3D-Au nanocomposite films. To improve the reversible switching effect, composites with MWCNTs instead of gold nanoparticles have also been tested and the results will be discussed.

DS 38.6 Thu 15:15 H8

Electrical properties of magnetron sputtered ZnO:Al samples determined by Hall and Seebeck measurements — •Wilma Dewald[1], Volker Sittinger[1], Bernd Szyszka[1], Mark Wimmer[2], and Florian Ruske[2] — [1]Fraunhofer Institute for Surface Engineering and Thin Films (IST), Bienroder Weg 54E, 38108 Braunschweig, Germany — [2]Helmholtz-Zentrum Berlin für Materialien und Energie (HZB), Kekuléstraße 5, 12489 Berlin, Germany

Transparent conductive oxides (TCOs) play a big role in display and photovoltaic technology. One of the most promising materials for photovoltaic applications is aluminum doped zinc oxide. The electrical properties of differently prepared ZnO:Al films will be analyzed in this paper.

Carrier mobility and free carrier density are varying in a wide range depending on the preparation method and doping level. Reactive mid frequency magnetron sputtering of a metallic Zn:Al target, radio frequency and direct current magnetron sputtering of a ceramic ZnO:Al$_2$O$_3$ target are considered as well as the post deposition annealing of samples, which increases mobility significantly. The carrier mobility in polycrystalline aluminum doped ZnO is limited by scattering at grain boundaries and at ionized impurities. With Hall and Seebeck measurements insight will be given in transport and scatter mechanisms for the different samples.

DS 38.7 Thu 15:30 H8

SnSe$_2$: An XAS study on the atomic and electronic structure — •Peter Zalden[1], Julia van Eijk[1], Carolin Braun[2], Wolfgang Bensch[2], Matthieu Micoulaut[3], and Matthias Wuttig[1] — [1]I. Physikalisches Institut (IA), RWTH Aachen, 52056 Aachen — [2]Institut für Anorganische Chemie, Univ. Kiel, 24118 Kiel — [3]Lab. de Physique Théorique de la Matière Condensée, UPMC, Paris 6

Phase-change materials (PCMs) show remarkable properties from a scientific and technological point of view: They are employed in non-volatile memory applications, while the general motif of the fast crystallization mechanism is still under investigation. Data storage with PCMs is based on different optical reflectivities and electronic resistivites of the metastable amorphous and crystalline phases. Although being employed in devices, several PCMs are chemically unstable, thus limiting the number of switching cycles.

In this study, SnSe$_2$, a rather uncommon candidate for PCMs has been investigated because of the stability of its crystalline and amorphous phases. Therefore, long data retention as compared to other PCMs should be possible. EXAFS measurements have been performed on both K absorption edges of the amorphous and crystalline phases, resulting in structural models for both phases. Although SnSe$_2$ has a small contrast in reflectivity, the electronic conductivity changes by several orders of magnitude. This might enable the application in case of a lower demand for write speed.

DS 38.8 Thu 15:45 H8

Preparation and characterization of CuCrO$_2$ — •Christina Polenzky, Kai Ortner, and Bernd Szyszka — Fraunhofer IST, Bienroder Weg 54E, 38108 Braunschweig, Germany

Transparent conductive oxides (TCOs) are promising materials for future application in the field of transparent electronics. The still existing lack of p-TCOs results from different reasons. Firstly, delafossites need high temperatures ($> 800\,^\circ$C) for crystallization which makes the coating difficult for most of the substrates used in industry. Secondly, as state of the art, the carrier concentration (n) and mobility (μ) are too low for suitable application.

In our work, we present results of the preparation and characterization of CuCrO$_2$. The synthesis of these materials from the gas phase by PVD will be demonstrated: The hollow cathode gas flow sputtering process is used for these materials for the first time. The dependency of the correct stoichiometry from gas flow and target composition is shown. Post-preparation annealing leads to better results by using a special atmosphere. So, the synthesis temperature is lowered for CuCrO$_2$ below 700 °C. CuCrO$_2$ shows p-type conductivity because of a positive Seebeck coefficient of $+477\ \mu$V/K. Furthermore, our delafossite materials reach transparencies up to 70 % in the visible spectrum of light.

With our work, we are able to improve the preparation of p-type TCOs and to bring them on the way into the future of transparent electronics.

DS 38.9 Thu 16:00 H8

Electrical transport in Al-doped ZnO/Ag/Al-doped ZnO multilayer systems — •Martin Philipp[1,2], Christian Hess[1], Hartmut Vinzelberg[1], Bernd Büchner[1], Hadia Gerardin[2], and Jacques Jupille[3] — [1]Leibnitz-Institute for Solid State and Materials Research IFW Dresden, 01171 Dresden, Germany — [2]Saint-Gobain Recherche, F-93303 Aubervilliers Cedex, France — [3]Institut des NanoSciences de Paris, Université Paris 6, CNRS UMR 7588, F-75015 Paris, France

Al-doped ZnO/Ag/Al-doped ZnO layer stacks are widely used as low-emissivity coatings for building glazing due to their high reflectance in the infrared and high transmittance in the visible spectrum. For a fundamental understanding of their physical properties the layer stacks, which were produced by magnetron sputtering, have been investigated by means of electrical transport and Hall effect measurements. The resistivity was measured in dependence of temperature and magnetic field on layer stacks of different silver film thicknesses. The results were analyzed using different thin film resistivity models in order to understand the basic scattering mechanisms inside the films. Furthermore the effect of annealing was studied.

DS 38.10 Thu 16:15 H8

Characterization of ion beam modified polyimide layers — •Daniel Friedrich[1], Marcel Michling[1], Dieter Schmeisser[1], Yuri Koval[2], and Paul Müller[2] — [1]Brandenburgische Technische Universität Cottbus, Angewandte Physik/Sensorik, K.- Wachsmann-Allee 1, 03046 Cottbus — [2]Universität Erlangen Nürnberg, Experimental Physik/Supraleitung, Erwin-Rommel-Str. 1, 91058 Erlangen

Ion beam modified polyimide show high conductivity. In our investigation we focus on the electronic structure and the element composition, in order to understand the mechanism of conductivity. In our experiments we use the methods NEXAFS and PES. The measurements were done at the U49/2-PGM2 beam line of BESSY II, Berlin. We find an increase of the sp2 hybridized graphite contribution, after low Ar^+ ion doses bombardment while the temperature of the samples is varied from 300 K to 650 K. In addition we follow the He^+ bombardment induced changes by in-situ monitoring of the O1s, N1s content in the polyimide films.

DS 38.11 Thu 16:30 H8

In-situ investigation of swift heavy ion beam induced dewetting of thin oxide films — •Wolfgang Bolse[1], Sankarakumar Amirthapandian[1,2], and Florian Schuchart[1] — [1]Institut für Halbleiteroptik und Funktionelle Grenzflächen, Universität Stuttgart — [2]on leave from: IGCAR, Kalpakkam, India

Recently we have reported dewetting of thin oxide films on Si during irradiation with swift heavy ions [1]. The dewetting patterns compared surprisingly well with those observed when melting polymer films on Si [2], although the irradiation was performed at 80 K, far below the melting point of the oxides. Hence, the dewetting processes and driving forces must be similar. In fact, we could identify the same hole nucleation mechanisms as reported for the polymers: heterogeneous nucleation at interfacial defects and spontaneous (homogeneous) nucleation due to (thermal) film density fluctuations. Using our new in-situ high resolution scanning electron microscope at the UNILAC accelerator of GSI, we are now able to follow the history of individual holes and determine their growth kinetics. In our first experiments we could show, that ion induced dewetting exhibits hole growth with rim formation, with the hole area being proportional to the applied ion fluence after the hole has fully evolved. This points at a growth mechanism which is controlled by the dissipation of the material removed from the hole. Capillary forces dominated growth (exponential increase with fluence) could be identified in the early stages of dewetting.

[1] T. Bolse, et al., Nucl. Instr. Meth. B 244 (2006) 113

[2] S. Herminghaus, et al., Science 282 (1998) 916

DS 39: Layer Deposition Processes & Layer Growth

Time: Thursday 17:00–18:00 Location: H8

DS 39.1 Thu 17:00 H8

Twin assisted growth of silicon on glass from low temperature solution and the onset of a morphological instability — •Robert Heimburger, Thomas Teubner, Nils Dessmann, Torsten Boeck, and Roberto Fornari — Leibniz–Institut für Kristallzüchtung, Max–Born–Straße 2, 12489 Berlin

Low temperature solution growth of microcrystalline silicon on glass substrates is considered in the light of supersaturation conditions and underlying growth mechanisms.

Silicon crystallites grown from liquid indium by means of steady–state solution growth at 600°C are terminated by $\{111\}$ facets. Often, individual grains consist of one or more $\Sigma3$ twin–boundaries. Alternating ledges and reentrant edges formed at multiple twin boundaries are found to locally enhance growth rate leading to anisotropic platelike structures. This can be explained by the presence of a self–preserving elementary step at the reentrant edges enabling fast growth even at low supersaturation without the need for 2D–nucleation. Additionally, if the size of a perfect crystal exceeds a certain value, the formation of hoppers in the middle of $\{111\}$ facets is observed. This morphological instability is interpreted by means of a supersaturation inhomogeneity arising within the diffusion boundary layer of the nutrient solution which causes solute depletion at the center of growing facets. As crystals exceed a critical size, this depletion cannot be longer compensated by an increased interstep distance. This leads to a significant decrease of growth rate at the centers.

DS 39.2 Thu 17:15 H8

Atomic layer deposition of HfO_2 onto SiO_2 substrates investigated in-situ by non-contact UHV/AFM — •Krzysztof Kolanek, Konstantin Karavaev, Massimo Tallarida, and Dieter Schmeisser — Brandenburgische Technische Universität, LS Angewandte Physik-Sensorik, Konrad-Wachsmann-Allee, 17, 03046, Cottbus, Germany

We investigated in-situ the atomic layer deposition (ALD) of HfO_2 onto SiO_2 substrates with ultra high vacuum (UHV) non-contact atomic force microscope (NC-AFM). The ALD process was started after detailed analysis of the initial Si(001)/SiO_2 substrate. The ALD cycles, made by using tetrakis-di-methyl-amido-Hf (TDMAHf) and water as precursors, were performed on the SiO_2 substrate maintained at 230 °C. We studied the relation between the film growth and the root mean square surface roughness, surface skewness, kurtosis, fractal dimension and correlation length. In the initial stages of the ALD process with our analysis of the surface height histograms we were capable of determination: HfO_2 layer thickness, surface coverage and surface roughness of a substrate and deposited material. Observation of the surface height histograms evolution during deposition allowed us to verify conformal and effective ALD growth on SiO_2 substrate. With this detailed analysis of the surface topography we confirmed the completion of the first HfO_2 layer after four ALD cycles.

DS 39.3 Thu 17:30 H8

Epitaxial growth of FeAl films on Al_2O_3 by pulsed laser deposition — •Moritz Trautvetter, Ulf Wiedwald, and Paul Ziemann — Institut für Festkörperphysik, Universität Ulm

FeAl alloys at equiatomic composition are very interesting systems due to their chemical stability and their multiple magnetic properties depending on chemical ordering. For many applications thin films are desirable. We present a method to grow epitaxial FeAl thin films on differently-cut sapphire (0001),$(11\bar{2}0)$,$(1\bar{1}02)$ substrates by pulsed laser deposition. By varying the preparation temperature, the film morphology can be tuned from very smooth films (300 K) to columnlike growth (900 K). Moreover, chemical ordering in the B2 structure can be achieved by film deposition at elevated temperatures or alternatively by post-annealing of smooth films deposited at ambient temperatures. The epitaxial relations were measured by X-ray diffraction and electron backscatter diffraction. The phase change from the bcc structure towards the B2 structure is accompanied by a ferromagnetic/paramagnetic phase transition. The magnetic properties of the different phases of the FeAl films are examined by SQUID magnetometry and AC-susceptibility.

DS 39.4 Thu 17:45 H8

Modeling of the relaxation kinetics of metastable tensile strained Si:C alloys — •Felix Ulomek[1], Ina Ostermay[2], Thorsten Kammler[3], and Volker Mohles[1] — [1]Institut für Metallkunde und Metallphysik, RWTH Aachen — [2]Fraunhofer-Center Nanoelektronische Technologien, Königsbrücker Straße 180, D-01099 Dresden — [3]GLOBALFOUNDRIES Dresden Module One LLC & Co. KG, Wilschdorfer Landstraße 101, 01109 Dresden

In order to enhance the performance of CMOS transistors, embedded epitaxial layers of Si:C can be used. In the present work, Si:C layers with Carbon contents up to 1.9 at-% and in-situ Phosphorus doping up to 4×10^{20} At/cm^3 have been investigated. Due to the low solubility of Carbon in Silicon (0.0004 at.-% at the melting point), all layers considered in this work are metastable and tend to relax. Since it is crucial to the application to retain the strain of those layers, the responsible mechanisms must be understood. The relaxation during thermal treatment was studied by high resolution X-ray diffraction and was found to behave differently, depending on Carbon content and Phosphorus doping concentration. In this work, we propose a relaxation mechanism based on a kick-out reaction of substitutional Carbon which is accelerated by Phosphorus content through transient enhanced diffusion. We simulate the time evolution of layer relaxation as a function of alloying content, layer thickness and temperature. Parameters for the reaction kinetics are obtained by fitting to the experimental data.

DS 40: [O] Plasmonics and Nanooptics V (Joint Session DS/O/HL)

Time: Thursday 10:30–13:00 Location: H32

DS 40.1 Thu 10:30 H32

Enhancing higher harmonics generation using plasmonic nanostructures — •Thomas Paul, Christoph Menzel, Carsten Rockstuhl, Shakeeb Bin Hasan, and Falk Lederer — Institute of Solid State Physics and Optics, Friedrich Schiller Universität Jena, Germany

Exploiting the properties of plasmon polaritons sustained by metallic nanostructures opens up great opportunities in engineering linear and nonlinear optical properties of conventional optical matter. Whereas the linear properties are usually at the focus of interest, also the nonlinear properties may benefit. If the metallic nanostructures are operated in resonance, the enhanced electrical field concentration facilitates the nonlinear interaction of light with matter. In our work we aim to detail such processes from a theoretical point of view. Particularly, we investigate the potential to enhance the higher harmonics generation by periodically arranged metallic nanostructures incorporated into a (nonlinear) dielectric host material. The geometries we are interested in are pairs of gold nanowires and split cylinder resonator structures. Emphasis is put on $\chi(2)$-nonlinearities for which it is reasonably assumed that the intrinsic nonlinearities of the dielectric host material prevails against those of the metallic nanostructures. Independent of the structure, we reveal the peculiarities of how the various types of resonances (dipolar or quadrupolar) may boost the conversion efficiency of the fundamental light into its higher harmonics (i.e. second harmonic). Possible implications to use the process of parametrical amplification for compensating absorption losses will be discussed.

DS 40.2 Thu 10:45 H32

Theoretical Investigation of the Electron Emission from Metal Nanotips — •Steve Lenk and Erich Runge — Institut für Physik und Institut für Mikro- und Nanotechnologien, Technische Universität Ilmenau, 98693 Ilmenau, Germany

We investigate the electron emission process from sharp metallic nanotips illuminated by low-power femtosecond laser pulses theoretically. The emission processes under discussion for few-femtosecond laser pulses are multiphoton emission [1] and optical field emission [2]. We calculate the probability current from a numerical solution of an initial value problem [3] via an exponential split-operator method and a real space product formula algorithm [4] in one and two spatial dimensions. The time-dependent electric potential used for the study of the electron emission is derived from the charge distribution on the tip apex. The electric field and the photoelectron current are compared with experimental results.

[1] C. Ropers, D. Solli, C. Schulz, C. Lienau, and T. Elsaesser, Phys. Rev. Lett. **98**, 043907 (2007).

[2] P. Hommelhoff, C. Kealhofer, and M. Kasevich, Phys. Rev. Lett. **97**, 247402 (2006).

[3] S. Glutsch, *Excitons in Low−Dimensional Semiconductors*, Springer Heidelberg (2004).

[4] H. De Raedt, Comp. Phys. Rep. **7**, 1 (1987).

DS 40.3 Thu 11:00 H32

Electromagnetic field enhancement at nanostructured surfaces — •Natalia Garcia Rey and Heike Arnolds — Surface Science Research Centre, University of Liverpool, Oxford Street, Liverpool L69 3BX, UK

Metal surfaces with nanometer scale roughness have been found to be photochemically more active than flat surfaces. This is believed to be caused by the excitation of surface plasmons, which create enhanced electromagnetic fields at the surface.

In this contribution, we explore the field enhancement obtainable from sub-wavelength periodic ripple structures created by argon ion sputtering in UHV, where we model the ripple surface structure as quasi-sinusoidal and solve Maxwell's equations in 2D with the help of finite-element modelling. We calculate the average surface field enhancement for various substrates (noble and transition metals) and vary incident wavelength and ripple periodicity and height.

Based on these results we discuss to which degree it is possible to maximize the electric field strengths and in turn the photochemical cross section using simple large-scale surface patterning techniques like sputtering.

DS 40.4 Thu 11:15 H32

Optical response of metallic nanostructures: simulation vs. measurement — •Reto Giannini[1], Patrick Leidenberger[2], Christian Hafner[2], and Jörg F. Löffler[1] — [1]Laboratory of Metal Physics and Technology, Department of Materials, ETH Zurich, 8093 Zurich, Switzerland — [2]Laboratory for Electromagnetic Fields and Microwave Electronics, ETH Zurich, 8092 Zurich, Switzerland

Today various different tools for calculating the optical response of metallic nanostructures are available. All of them are based on a geometric description of the nanostructures, which makes it difficult to take into account production-based variations in the shape of the structure under investigation. In the context of plasmon resonances in the optical wavelength range and related effects, such as field enhancement, this discrepancy can generate significant deviations between simulation and measurement. To address this problem, we performed a series of FEM-based simulations on Au-nanoparticles, aiming to approach as closely as possible the structures available using today's state-of-the art production techniques. The simulations were carried out using JCMsuite (axis-symmetric model) and Comsol (full 3D), and special attention was paid to corners, triple-points and particle deformation. The calculated results were then compared with nanoparticles produced and analyzed in-house.

DS 40.5 Thu 11:30 H32

Modeling Metallic Nanostructures using a Discontinuous Galerkin Approach — •Jens Niegemann[1,2], Michael König[1,2], Richard Diehl[1], Christopher Prohm[1], and Kurt Busch[1,2] — [1]Institut für Theoretische Festkörperphysik, Karlsruher Institut für Technologie — [2]DFG Forschungszentrum Center for Functional Nanostructures (CFN), Karlsruher Institut für Technologie

Over the past few years, the discontinuous Galerkin time-domain (DGTD) method has established itself as an extremely powerful and efficient numerical technique in the field of photonic. Due to its combination of an accurate spatial discretization with an explicit time-stepping scheme, the DGTD method is particularly well suited for studying ultra-short and/or plasmonic phenomena.

Here, we present our recent advances in using the DGTD method for the simulation of metallic nanostructures. In particular, we present the advantages of using higher-order curved elements. Furthermore, we will discuss some of our recent developments with respect to the improvement of the time integration.

DS 40.6 Thu 11:45 H32

Mode Tuning in Microresonators Using Uniaxial Anisotropy

and Resonator Shaping — •Stefan Declair, Cedrik Meier, Torsten Meier, and Jens Förstner — University of Paderborn, Department of Physics and CeOPP, Warburger Str. 100, D-33098 Paderborn, Germany

We numerically investigate resonant modes in microdisks and photonic crystal cavities. Mode tuning of the resonant modes, which is desirable for many applications, e.g. for achieving strong coupling, in a broad frequency range is shown using (a) uniaxial anisotropy of either the surrounding environment or the photonic structure and (b) in non-cylindrical microdisks. In both cases anticrossing behavior is observed when modes of different mode order approach each other. Additionally, we compare our simulations with experimental results from a 3 μm microdisk embedded in a liquid crystal environment.

DS 40.7 Thu 12:00 H32

Microcavity Plasmonics — •Ralf Ameling and Harald Giessen — 4th Physics Institute, University of Stuttgart, Germany

We couple hybridized plasmon modes in cut-wire metamaterials with resonator modes of a microcavity. Depending on the position of the cut-wire pair in the resonator, the symmetric (electric) or antisymmetric (magnetic) plasmon mode is coupled, manifested by an anticrossing of the resonances. We explain this behavior by taking the symmetry and spatial distribution of the electric fields in the resonator into account. Experimental results verify the predicted mode-splitting due to the strong resonant coupling and agree well with theory. Our work can serve as a model system for far-field plasmon-plasmon coupling and paves the way towards enhanced plasmon-plasmon interaction in photonically coupled three-dimensional Bragg structures.

DS 40.8 Thu 12:15 H32

Functional elements on subwavelength plasmonic waveguides — •Andreas Reiserer[1], Philip Tuchscherer[1], Christian Rewitz[1], Dmitri V. Voronine[1], Jer-Shing Huang[2], Bert Hecht[2], and Tobias Brixner[1] — [1]Institut für Physikalische Chemie, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany — [2]Nano-Optics and Biophotonics Group, Physikalisches Institut, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany

Plasmonic functional elements are promising to combine the advantages of photonics and electronics – high speed and small spatial extent. We employ numerical simulations and an analytic approach based on transmission line theory to demonstrate several functional elements that consist of so called stub structures – terminated ends on metal–insulator–metal waveguides.

Splitters are presented that allow arbitrary adjustment of the transmission ratio from an input to two different output arms; frequency filters are designed that provide steep transmission resonances; and, finally, nanoscale all-plasmonic switching is proposed with an operating frequency of more than 20 THz.

The suggested device components are promising for future applications in ultrafast nanoscale information processing.

DS 40.9 Thu 12:30 H32

Optimally Shaped Laser Pulses for Hybrid Metal-Semiconductor Nanostructures — •Matthias Reichelt[1], Torsten Meier[1], Andrea Walther[2], and Michael Dellnitz[2] — [1]Department Physik, Universität Paderborn, Warburger Str. 100, D-33098 Paderborn, Germany — [2]Institut für Mathematik, Universität Paderborn, Warburger Str. 100, D-33098 Paderborn, Germany

A hybrid nanostructure which consists of a metal aperture and a semiconductor quantum wire is studied theoretically. [1] It is shown that one can concentrate the optically excited electron density at an arbitray position for a given time using sophistically shaped laser pulses. To obtain the optimized laser field a genetic algorithm [2] and a more rigorous mathematical approach [3] are applied. Full three-dimensional finite-difference time-domain calculations [4] confirm the predicted spatiotemporal control.

[1] M. Reichelt and T. Meier, Opt. Lett. **34**, 2900 (2009).
[2] A.E. Eiben and J.E. Smith, *Introduction to Evolutionary Computing*, Springer (2003)
[3] S. Sertl and M. Dellnitz, Journal of Global Optimization **34**, 569-587, (2006).
[4] A. Taflove, *Advances in Computational Electrodynamics*, Artech House, (1998).

DS 40.10 Thu 12:45 H32

Analytic Theory of Linear Plasmonic Antennas — Jens Dorfmüller[1], Ralf Vogelgesang[1], •Moritz Esslinger[1], Worawut Khunsin[1], Christian Ettrich[2], Carsten Rockstuhl[2], and Klaus Kern[1] — [1]Max Planck Institute for Solid State Research, 70569 Stuttgart, Germany — [2]Institute of Condensed Matter Theory and Solid State Optics, Friedrich-Schiller Universität Jena

At radio-frequencies, antenna theory is a well understood topic. At optical frequencies, however, antenna sizes are in the order of skin depths so that electromagnetic fields penetrate substantially into the volume of metallic nanostructures, rendering classic radio antenna theory not applicable. We develop a fully analytical model for the electromagnetic behavior of plasmonic wires. Therefore, we model thin, linear plasmonic antennas based on the assumption of homogeneous volume currents. Our model requires only a handful, physically motivated, adjustable parameters. It successfully predicts measured and simulated data in full detail: emission patterns, nearfield optical amplitudes and phases, as well geometric resonances.

DS 41: [O] Plasmonics and Nanooptics VI (Joint Session DS/O/HL)

Time: Thursday 15:00–18:00 Location: H32

DS 41.1 Thu 15:00 H32

Surface plasmon polaritons on arrays of nanostructures with three-fold symmetry — •David Leipold, Stephan Schwieger, and Erich Runge — Institut für Physik und Institut für Mikro- und Nanotechnologien, Technische Universität Ilmenau

Surface plasmon polaritons (SPPs) are optical excitations that are confined to a metal-dielectric interface. They interact with propagating light if the metal is structured on the scale of the wavelength of the incident light. Here, we consider the coupling properties of quadratic arrays of nano-holes cut into a silver film. In particular, we investigate the influence of nano-holes with three-fold symmetry, which is incompatible with the four-fold symmetry of the array. Our numerical results reproduce aspects of earlier experimental findings [1]. Namely, there are shifts in the SPP-related minima and maxima in the reflectivity of specific reflection orders as function of the polarization of the incident light.

[1] B. Ashall, M. Berndt, and D. Zerulla, *App. Phys. Lett.* **91**, 203109 (2007)

DS 41.2 Thu 15:15 H32

Determination of surface plasmon polariton velocity measured by scattering scanning nearfield optical microscopy — •Brian Ashall and Dominic Zerulla — School of Physics, University College Dublin, Dublin 4, Ireland.

Surface Plasmon Polaritons (SPPs) are electromagnetic waves, propagating at the interface of a metal and a dielectric material, that are coupled to a charge density oscillation of the free electrons of the metal. In order to examine the optical nearfields of SPPs as they interact with nanoscale topography features, the technique of scattering Scanning Nearfield Optical Microscopy (sSNOM) is used. Presented here is an example of direct imaging of standing SPP interference patterns following interaction with a sharp topographic reflector. Analysis of this SPP interference pattern demonstrates a SPP propagation velocity of 0.93 times the speed of light. In addition to this, interaction of SPPs with specifically designed surface patterns will be demonstrated to yield a focussing of the plasmon nearfield.

DS 41.3 Thu 15:30 H32

Surface Plasmon Mapping using Photoelectron Emission Microscopy combined with Huygens principle — •Christian Schneider, Alexander Fischer, Martin Rohmer, Daniela Bayer, Pascal Melchior, and Martin Aeschlimann — Department of Physics and Research Center OPTIMAS, University of Kaiserslautern, 67663 Kaiserslautern

Photoelectron emission microscopy (PEEM) is a very powerful tool to investigate electron dynamics simultaneously in time and space with femtosecond temporal and nanometer spatial resolution. This microscopy technique is also suitable to study plasmonic behaviour in metal nanostructures, which combines the advantages of photonics and electronics. In this talk, we will show PEEM measurements of structures exhibiting surface plasmon polariton (SPP) resonances and present a novel simulation method based on Huygens' principle. As only the beating between the exciting light wave and the SPP wave can be observed by PEEM, a direct access to the surface plasmon wave isn't possible. Applying the simple wave model of Huygens in combination with a fast and reliable fitting algorithm to the complex PEEM data allows us to recalculate the propagating SPP wave for different shaped nanostructures. Examples like gold-squares as well as L-shaped structures are presented.

DS 41.4 Thu 15:45 H32

Photoemission Microscopy with Surface Plasmon Polaritons — Niemma Buckanie[1], Nicolai Rass[1,2], Pierre Kirschbaum[1], Michael Horn-von Hoegen[1], and •Frank-J. Meyer zu Heringdorf[1] — [1]Universität Duisburg-Essen, Fakultät für Physik and Center for Nanointegration (CeNIDE), Lotharstrasse 1, 47057 Duisburg, Germany — [2]present address: E.ON Gastransport GmbH, 45141 Essen, Germany

The interaction of frequency doubled femtosecond laser pulses with Silver provides a fantastic opportunity to study surface plasmon polariton (SPP) phenomena in Ag nanostructures. In two photon photoemission microscopy (2PPE PEEM) using femtosecond laser pulses, SPPs are imaged as a superposition of the electric field of the travelling SPP wave with the electric field of the laser pulse that hits the surface under grazing incidence. As the SPP and the fs laser pulse travel at different speeds, a moiré pattern is formed across the island that can be directly imaged in 2PPE PEEM. The period and orientation of the moiré pattern are influenced by the angle between the propagation direction of the SPP wave and the projection of the direction of incidence of the laser pulse into the surface plane. In a pump-probe experiment, where two coherent fs laser pulses are mutually time-delayed, it is possible to shift the moiré pattern across the island, to visualize the propagation of the SPP, and to control the location of maximum intensity behind the particle.

DS 41.5 Thu 16:00 H32

Free-Space Excitation of Propagating Surface Plasmon Polaritons — •Jan Renger[1], Romain Quidant[1], Niek van Hulst[1], Stefano Palomba[2], and Lukas Novotny[2] — [1]ICFO-Institut de Ciencies Fotoniques, 08860 Castelldefels (Barcelona), Spain — [2]Institute of Optics, University of Rochester, Rochester, NY 14627, USA

A unique feature of surface plasmon polaritons (SPPs) is that their in-plane momentum is larger than the momentum of free-propagating photons of the same energy. Therefore, it is believed that they can be excited only by evanescent fields created by total internal refection or by local scattering. Here, we provide the first demonstration of free-space excitation of surface plasmons by means of nonlinear four-wave mixing [1]. The process involves the vectorial addition of the momenta of three incident photons, making it possible to penetrate the light cone and directly couple to the SPP dispersion curve. Using this technique, surface plasmons can be launched on any metal surface by simply overlapping two beams of laser pulses incident from resonant directions. The excitation scheme is also applicable to other bound modes, such as waveguide modes, surface phonon-polaritons, and excitations of two-dimensional electron gases. [1] J. Renger et al. Phys. Rev. Lett. accepted (2009)

DS 41.6 Thu 16:15 H32

Femtosecond Surface Plasmon Characterisation on Metallic Dielectric Interfaces — Jose Francisco Lopez-Barbera, Brian Ashall, and •Dominic Zerulla — University College Dublin, School of Physics, Dublin 4, Ireland

As result of the latest advances in ultrashort pulse measurements, it is now possible to investigate ultrashort processes such as surface plasmon polariton (SPP) dynamics on a sub 20 fs time scale. SPPs are one of the fastest events in nature with time scales varying from 100s of attoseconds to 100s of nanoseconds. Using advanced autocorrelation techniques based on optical gating (FROG and GRENOUILLE) in combination with a 12 fs broadband Ti:Sa laser system, we have characterised the resonant photon-SPP coupling processes on metallic thin films. In particular we focus on the excitation, propagation and life-time of the SPPs at high temporal and frequency resolution. We will present surprising insights into the behaviour of SPPs on this short timescales, including data on the interference of the SPP emission with the directly reflected/diffracted channel.

DS 41.7 Thu 16:30 H32

Light guiding in para-hexaphenylene based nanofibers in interaction with a gold substrate studied by photoemission electron microcopy — •Till Leissner[1], Michael Bauer[1], Kasper Thilsing-Hansen[2], Roana Melina de Oliveira Hansen[2], Jakob Kjelstrup-Hansen[2], and Horst-Günther Rubahn[2] — [1]Institut für Experimentelle und Angewandte Physik, Universität Kiel — [2]NanoSYD, Mads Clausen Institute, University of Southern Denmark

Para-hexaphenylene (p-6P) based nanofibers have been proven to support almost loss-free and broadband optical wave guiding up to wavelengths as short as 400 nm [1]. As a dielectric distortion on top of a metallic substrate, they can, additionally, support the localized propagating of interface plasmon modes. P-6P nanofibers may therefore be useful as light-channeling sub-units and highly localized emitters in future ultrafast nanophotonic devices. To address the interaction between optical waveguiding and surface plasmon excitations we deposited well aligned p-6P nanofibers onto microstructured gold films. Photoemission Electron Microscopy was used to image the local light modes excited by a femtosecond laser pulse. Within the nanofibers, periodic beating patterns are observed which exhibit a strong dependence on the polarization the excitation laser field. The pattern periodicity can quantitatively be modeled and assigned to the interference between a propagating interface plasmon and the excitation light field, thus given evidence for plasmon guiding by the nanofibers.

[1] H.-G. Rubahn et al., Appl. Phys. Lett. 82, 10 (2003)

DS 41.8 Thu 16:45 H32

Surface Plasmon Excitation on Magnetoactive Hybrid Materials — •Dominic Zerulla and Brian Ashall — UCD Dublin, School of Physics, Dublin 4, Ireland

The interaction of surface plasmons polaritons (SPPs) - fluctuations in the electron density at the interface between media with dielectric constants of opposite sign - with magnetically ordered systems has attracted a significant interest in recent years, as a result of the possibility of enhancing magneto-optical properties, like the Faraday and Kerr effect. More recently, research has been focused on the merging of the areas of spintronics and plasmonics, thus developing a new field called spin-plasmonics. Here, we will present a systematic study of the excitation of SPPs on ferromagnetic materials in multilayered structures composed of thin films of nickel, iron, cobalt, capped by a silver layer [1]. The electromagnetic properties of the systems are theoretically and experimentally investigated as a function of the metal layers' thickness and the critical parameters in this study of the interaction between surface plasmon waves and the magneto-active material are discussed. Finally, an optimized structure for the investigations of spin-plasmonic effects in thin films is proposed.

[1] L. Sapienza, D. Zerulla, "Surface Plasmon Excitation on Magnetoactive Materials", Phys. Rev. B 79, 033407 (2009)

DS 41.9 Thu 17:00 H32

Loss compensation of surface plasmon polaritons in multilayer structures with optically pumped gain media — Patrick Scholz[1,2], •Stephan Schwieger[1], and Erich Runge[1] — [1]Institut für Physik and Institut für Mikro- und Nanotechnologien, Technische Universität Ilmenau, 98693 Ilmenau, Germany — [2]Climate Science Division, Alfred Wegener Institut für Polar- und Meeresforschung, 27570 Bremerhaven, Germany

Surface plasmon polaritons (SPPs) that are excited at metal gratings have large losses due to metallic absorption and re-radiation into propagating far-field modes. These losses can be possibly compensated by energy transfer from thin layers of optically excited media, such as semiconductor quantum wells in close vicinity to the metal surface [1,2]. In this contribution, the loss compensation is investigated theoretically as a function of the geometry of the sample. Parameters, such as the grating period, the slit width, the thickness of the metal film, and the spatial separation between the quantum well and the metal are varied. Furthermore, the formation of coupled SPP-exciton modes and some of their properties, as, e.g., their life times, propagation lengths, and group velocities, are discussed.

[1] P. Vasa, R. Pomraenke, S. Schwieger, Yu. I. Mazur, Vas. Kunets, P. Srinivasan, E. Johnson, J. E. Kihm, D. S. Kim, E. Runge, G.

Salamo, and C. Lienau, *Phys. Rev. Lett.* **101**, 116801 (2008).
[2] S. Schwieger, P. Vasa, and E. Runge, *Phys. Stat. Sol. (b)* **245**, 1071(2008).

DS 41.10 Thu 17:15 H32

Electrically influencing the surface plasmon dispersion relation — •Brian Ashall[1], Michael Berndt[2], and Dominic Zerulla[1] — [1]School of Physics, University College Dublin, Dublin 4, Ireland. — [2]Max Planck Institute of Molecular Cell Biology and Genetics, 01307 Dresden, Germany.

Surface Plasmon Polaritons (SPPs) are a resonant coupling of electromagnetic radiation to charge density oscillations of the conduction electrons at the surface of a metal. As this SPP charge density oscillation is based on electron movement, it is intuitive to consider the possibility of influencing SPPs with an applied electric current, which also moves the charges to which the SPPs are coupled. This possibility to directly influence SPPs is examined experimentally, along with indirect electrical influences, such as electric Joule heating. Additionally, the inverse process is examined; i.e. the potential for the creation of a direct net movement of electrons by propagating SPPs. The possibility for this to occur is supported by the fact that the electromagnetic waves describing SPPs possess electrical field components along the propagation direction of the plasmons, and so they should have some potential to move the charge carriers to which they are coupled.

DS 41.11 Thu 17:30 H32

Efficient Coupling of Single NV Centres to Surface Plasmon Polaritons — •Bernhard Grotz[1], Merle Becker[1], Sebastian Macke[2], Julia Tisler[1], Gopalakrishnan Balasubramanian[1], Fedor Jelezko[1], and Jörg Wrachtrup[1] — [1]3. Physikalisches Institut, Universität Stuttgart, Germany — [2]Max-Planck-Institut für Metallforschung, Stuttgart, Germany

When light interacts with metal surfaces it excites electrons which can form propagating charge-density waves called surface plasmon polaritons. These collective electronic excitations have many applications due to their ability to produce strong electric fields localized to subwavelength distance scales. It was shown that nanodiamonds containing single nitrogen-vacancy (NV)centres can be attached efficiently to silver nanowires where they are used to excite single surface plasmon polaritons [1]. We discuss recent approaches to address this problem and in particular how to increase the coupling strength between NV and nanowires.

[1] R. Kolesov, B. Grotz, G. Balasubramanian, R. J. Stöhr, A. A. L. Nicolet, P. R. Hemmer, F. Jelezko & J. Wrachtrup, Wave-particle duality of single surface plasmon polaritons, Nature Physics 5, 470-474 (2009)

DS 41.12 Thu 17:45 H32

Plasmonic Collimation for near-IR Laser Diodes — •Xinghui Yin[1,2], Justin White[3], Mark Brongersma[3], and Thomas Taubner[1,2] — [1]RWTH Aachen — [2]Fraunhofer-Institut für Lasertechnik — [3]Stanford University

It is known that one can use gratings to couple freely-propagating light to plasmon modes. Ebbesen [1] examined the reverse process at a metallic slit-grating structure and discovered a beaming effect. Subsequently, Capasso [2] successfully combined such a structure with a Quantum Cascade Laser at a mid-infrared wavelength of $\lambda = 9.8$ μm to reduce the beam divergence in one direction.

In our work, we investigate plasmonic collimators for laser diodes at near-infrared wavelengths. We focus on optimizing the structure parameters for $\lambda = 960$ nm. In this region, it is important to take the higher surface plasmon propagation losses into consideration. Also, we examine the efficiency of plasmonic collimation compared to conventional laser diode collimation by cylindric lenses.

The simulations are carried out using a 2D Finite Difference Frequency Domain code developed by J. White. Using the obtained parameters, we fabricate the plasmonic collimator and characterize it.

[1] Ebbesen et al., 2002, Vol 297, Science
[2] Capasso et al., Nature Photonics, 2008

DS 42: Invited Roke

Time: Friday 10:15–11:00 Location: H2

Invited Talk DS 42.1 Fri 10:15 H2

A molecular view of the interfaces of colloidal particles and nanoscopic oil droplets in water — •Sylvie Roke — Max-Planck Institute for Metals Research HeisenMax-Planck Institute for Metals Research , Heisenbergstrasse 3, 70569 Stuttgart, Germany

Second harmonic and sum frequency scattering spectroscopy offer a unique way of obtaining molecular information (chemical composition, molecular orientation, order and chirality) of the interfaces of micro- and nanoscopic particles in a solution or in a solid matrix. These methods can be used to monitor the colloidal interfacial structure and changes therein (e.g. change in molecular order or charging). In this presentation I will start with a description of the scattering methods and show how molecular surface effects can be extracted from the scattered frequency domain spectrum and its angular distribution. Finally we show measurements on nanoscopic oil-in-water droplets that show how surfactants sit at the droplet oil-water interface and that these interfaces are very different from equivalent planar interfaces.

DS 43: Biomolecular and Functional Organic Layers II (Focused Session)

Time: Friday 11:15–14:00 Location: H2

Topical Talk DS 43.1 Fri 11:15 H2

High resolution studies of bio-molecules using TERS — •Volker Deckert — Friedrich-Schiller-Universität, Jena, Deutschland — Institut für Photonische Technologien, Jena, Deutschland

Tip enhanced Raman scattering (TERS) is an adaption of the well established surface enhanced Raman spetroscopy (SERS) technique. TERS combines in a unique way the high sensitivity related to the field enhancing properties of SERS and the high lateral resolution capabilities of scanning probe microscopy, in particular near-field optical microscopy and allows a lateral resolution far beyond the Abbe limit.

With respect to the analysis of biomolecules, the aspect of a label-free sequencing of nucleic acid or amino acid based polymers is probably the most intriguing. TERS investigations of nano crystals of single nucleobases already proved the possibility to distinguish between the four bases and has recently been applied onto a single RNA strand. A further challenge is the application towards peptide characterization for this purpose special gold and silver substrates have been developed that allow the immobilization of the substrates without interfering with the signal intensities. Nevertheless, at first glance comparison with standard Raman and SERS experiments show an intriguing difference in the appearance of the spectra. It will be shown that this can now be readily explained by specific polarization properties of the TERS probe.

DS 43.2 Fri 11:45 H2

Electrochromic Redox Reactions of Highly Fluorinated Phthalocyanine Thin Films — •Stefanie Nagel[1], Christopher Keil[1], Sergiu Gorun[2], Robert Gerdes[2], and Derck Schlettwein[1] — [1]Institute of Applied Physics, Justus-Liebig-University Giessen, Germany. email:schlettwein@uni-giessen.de — [2]Department of Chemistry and Environmental Science, New Jersey Institute of Technology, Newark, NJ 07102, USA

Vacuum-evaporated thin films (10 - 100 nm) of copper complexes of hexadecafluorophthalocyanine ($F_{16}PcCu$) and octaperfluoro(isopropyl)phthalocyanine ($F_{64}PcCu$) on indium tin oxide electrodes have been studied in contact to $LiCl$ aqueous electrolyte by cyclic voltammetry. Simultaneous monitoring of the absorption spectra of the films reveals nearly reversible electrochromic behavior after some conditioning cycles caused by an irreversible structural change. Only one reduction and reoxidation peak can be observed. Different isosbestic points in different potential ranges indicate different reduced species. Electroneutrality of the films is preserved by intercalation of Li^+ ions. The influence of different film thickness and sweep rates on the cyclic voltammetry and spectral changes has been investigated. Due to the electron withdrawing effect of the substituents the redox potential is found to be shifted by about 0.2 V for $F_{64}PcCu$ towards more positive potentials relative to $F_{16}PcCu$. An increase of intermolecular coupling in $F_{16}PcCu$ compared with $F_{64}PcCu$ is concluded from an observed spectral broadening of the Q-band.

DS 43.3 Fri 12:00 H2

Monitoring photooxidation of acetone on TiO_2(110) using IR spectroscopy — •Youkun Gao[1], Mingchun Xu[1], Yuemin Wang[1], and Christof Wöll[2] — [1]Lehrstuhl für Physikalische Chemie I, Ruhr-Universität Bochum, 44801 Bochum, Germany — [2]Institut für Funktionelle Grenzflächen (IFG), Karlsruher Institut für Technologie, 76021 Karlsruhe, Germany

The photochemistry on semiconductor TiO_2 surfaces has recently received enormous attention from both fundamental and technological perspectives because of its extensive applications related to energy conversion and other associated processes with environmental impact. There is much interest in the heterogeneous photooxidation of acetone on TiO_2. Whereas acetone photooxidation has been extensively studied on TiO_2 powder samples there is, due to experimental difficulties, a general lack of information on single-crystal surfaces. In this work, we report the first IR studies of acetone photoreactions on the TiO_2(110) surface using reflection-absorption infrared spectroscopy (RAIRS). Exposing TiO_2 to acetone at 110 K leads to molecular (associatve) adsorption, forming mono- and multilayers. The dark reaction of acetone with oxygen molecules on this TiO_2 surface leads to the formation of η^2- diolate species. Irradiation with UV light leads to a conversion of this species to acetate via methyl radical ejection. Furthermore, we found that carbonate/bicarbonate is the final oxidation product after extended exposure to UV light. Finally, the quantum yield and photo-reaction cross section Q for photo-induced oxidation of acetone on differently modified TiO_2(110) surfaces were determined.

Topical Talk DS 43.4 Fri 12:15 H2

Molecular orientation in phthalocyanine films assessed by combined optical and magneto-optical investigations — •Georgeta Salvan[1], Michael Fronk[1], Björn Bräuer[1,2], Dietrich R. T. Zahn[1], Oliver G. Schmidt[3], and Jens Kortus[4] — [1]Chemnitz University of Technology, Physics Department, D-09107 Chemnitz, Germany — [2]SIMES Center, SLAC National Accelerator Laboratory, Stanford University, Stanford, CA 94309, USA — [3]Institute for Integrative Nanosciences, IFW Dresden, Helmholtzstr. 20, 01069 Dresden, Germany — [4]TU Bergakademie Freiberg, Theoretical Physics Department, D-09596 Freiberg, Germany

Magneto-optical Kerr effect (MOKE) is commonly used to study the magnetic properties of inorganic ferromagnetic layers or magnetic nanostructures. For the example of phthalocyanine thin films it will be shown that also paramagnetic and diamagnetic molecules can exhibit a strong MOKE signal in the visible to near ultraviolet spectral range. A numerical analysis of the energy dispersion of the real and imaginary part of the complex magneto-optical Kerr rotation angle and of the optical constants allows the determination of the magneto-optical material constant, the so-called Voigt constant. For phthalocyanines this is only about two orders of magnitude smaller compared to soft ferromagnetic materials such as Ni. The magnitude of the Voigt constant is found to be highly sensitive to the orientation of the molecules with respect to the substrate plane. This opens new possibilities to accurately determine the molecular orientation in organic thin films.

DS 43.5 Fri 12:45 H2

Environment-friendly photolithography using poly-(N-isopropylacrylamide)-based thermoresponsive photoresists — •Leonid Ionov[1], Nikolay Puretskiy[1], Georgy Stoychev[1], Svetlana Zakharchenko[1], Stefan Diez[2], and Manfred Stamm[1] — [1]Leibniz-Institut fuer Polymerforschung Dresden e.V., Dresden, Germany — [2]Max-Planck-Institute of Molecular Cell Biology and Genetics, Dresden, Germany

We report a novel approach for the temperature-triggered development of water-soluble photoresists based on photocleavable poly-(N-isopropylacrylamide) copolymers. These copolymers are soluble in aqueous environment below their Lower Critical Solution Temperature (LCST). Upon UV irradiation, the photocleavable groups are deprotected resulting in an increased LCST. Thus, the illuminated parts of spin-coated copolymer layers dissolve at higher temperatures than the surrounding areas, leading to pattern development. The photoresist can finally be completely removed at low temperature. We demonstrate the applicability of this novel photolithographic approach by the patterning of fluorescent proteins.

DS 43.6 Fri 13:00 H2

Avidin immobilization on mixed monomolecular template prepared by irradiation promoted exchange reaction — Nirmalya Ballav[1], Andreas Terfort[2], and •Michael Zharnikov[1] — [1]Angewandte Physikalische Chemie, Universität Heidelberg, 69120 Heidelberg, Germany — [2]Institut für Anorganische und Analytische Chemie, Goethe-Universität Frankfurt, Germany

An applicability of irradiation-promoted exchange reaction (IPER) to the fabrication of mixed self-assembled monolayers (SAMs) comprised of the protein-repelling matrix and moieties bearing binding sites for specific attachment of a target protein is demonstrated. As test systems, we took mixed films of oligoethyleneglycol (OEG) substituted alkanethiols (OEG-ATs) and biotin-substituted alkanethiols (BATs) on Au(111). Such SAMs are suitable for specific immobilization of avidin and its variants. The SAM composition was precisely controlled by varying the irradiation dose, which is a prerequisite for the fabrication of the respective patterns by electron-beam lithography. While the general trend in the immobilization of avidin onto the mixed OEG-AT/BAT SAMs prepared by IPER was found to be consistent with the earlier reports regarding the analogous films fabricated by the co-assembly method, the concentration of the BAT component in the mixed SAMs needed for the maximum surface coverage of the specific protein was found to be lower and the maximum avidin coverage higher in the case of IPER than for the co-assembly method. We ascribe these differences to the lack of phase segregation and better separation of the BAT species in the OEG-AT matrix in the case of IPER.

DS 43.7 Fri 13:15 H2

Structural Characterization of Self-assembled Monolayers of Pyridine-terminated Thiolates on Gold — •Jinxuan Liu[1], Björn Schüpbach[2], Asif Bashir[3], Osama Shekhah[1], Alexei Nefedov[1], Martin Kind[1], Andreas Terfort[2], and Christof Wöll[4] — [1]Lehrstuhl für Physikalische Chemie I, Ruhr-Universität Bochum, 44780 Bochum, Germany — [2]Institut für Anorganische und Analytische Chemie, Goethe-Universität Frankfurt am Main, 60325 Frankfurt, Germany — [3]Interface Chemistry and Surface Engineering, Max-Planck-Institut für Eisenforschung, 40237 Düsseldorf, Germany — [4]Institute of Functional Interfaces, Karlsruhe Institute of Technology (KIT), 76021 Karlsruhe, Germany

Self-assembled monolayers (SAMs) on Au from a homologous series of four pyridine-terminated organo thiols have been investigated using a variety of surface-analytical techniques (IR, XPS, NEXAFS, STM) and DFT calculations. For all pyridine-terminated thiols the immersion of Au-substrates in the corresponding ethanolic solutions was found to result in the formation of highly ordered and densely packed SAMs. For an even number of the methylene spacers between the SH group and the aromatic moieties the SAM unit-cell is rather large, $5\sqrt{3} \times 3$, whereas in case of an odd number of methylene units a smaller unit cell is adopted, $2\sqrt{3} \times \sqrt{3}$ R30°. The tilt-angle of the molecules amounts to 15°. In contrast to expectation, the pyridine-terminated organic surfaces exposed by the corresponding SAMs showed a surprisingly strong resistance with regard to protonation.

Topical Talk DS 43.8 Fri 13:30 H2

***In-silico* optimization of function and emissive properties of Silicon nanoparticles** — •Thomas Niehaus — Bremen Center for Computational Materials Science, Bremen, Germany

Excited-state properties of silicon quantum dots (SiQDs) up to diameters of 2 nm are studied using an approximate time-dependent density-functional theory method (TD-DFTB) [1] and compared with available experimental data. Several functionalizations ranging from simple hydrogen passivation up to capping with amine [2], allyamine [3] and propionic acid [4] groups are discussed. Signatures in vibrational and optical absorption spectra are revealed, which show the detailed effect of surface modification of the SiQDs. It is verified that the modification could be expected to not only reduce the surface oxidation rate but also maintain an efficient electronic transition feature that facilitates blue emission. The obtained absorption spectra show a significant size dependence. In the case of allylamine capping, the increase in the number of attached molecules only results in a slight red shift of emission spectra. The latter are calculated by means of full geometry optimization in the excited state and reveal huge Stoke shifts in contrast to simple quantum confinement models [5].

[1] T.A. Niehaus et al., Phys. Rev. B, 63, 085108, 2001. [2] Q.S. Li et al., Appl. Phys. Lett., 92, 053107, 2008. [3] X. Wang et al., J. Phys. Chem. C, 111, 2394, 2007. [4] Q.S. Li et al., J. Chem. Theo. Comp., 3, 1518, 2007. [5] X. Wang et al., Appl. Phys. Lett., 90, 123116, 2007.

DS 44: Organic Thin Films I

Time: Friday 10:15–11:45 Location: H8

DS 44.1 Fri 10:15 H8

Charge Transport Investigation in Organic Semiconductors by Electro-Reflectance — •Steve Pittner and Veit Wagner — School of Engineering, Jacobs University Bremen, Campus Ring 1, D-28759 Bremen, Germany

Organic semiconductors have proven to be suitable materials for electronic devices, such as organic solar cells, organic field effect transistors (OFET), and organic light emitting diodes. Generally organic semiconductors exhibit rather low charge mobility and it is crucial to understand the details of charge transport within organic material for further improvements. Disordered organic materials often exhibit a charge carrier density dependent mobility (see e.g. Vissenberg/Matters) and the aim of this work is to analyse the contribution of carriers with different mobilities during the electrical charge transport between electrodes. For this purpose the spectral fingerprint of the charge carriers under investigation is detected locally by electro-modulation spectroscopy. This is done in an OFET-like geometry with an applied alternating voltage. Clear changes of the fingerprint spectrum with the DC gate voltage as well as with the lateral distance to an electrode are detected. The changes occur at a photon energy around 1.9 eV for a poly(3-hexylthiophene) (P3HT) semiconducting layer. The depletion of the high energy shoulder clearly reflects the charge carrier population modification with gate voltage and/or distance to the injecting electrode. The changes are interpreted as time-dependent settling of the injected charge carriers to lower energy polaronic states related to the band tails of the material.

DS 44.2 Fri 10:30 H8

Simultaneous in-situ real-time measurements of X-ray reflectivity and optical spectra of organic semiconductor thin film during growth — •Takuya Hosokai, Alexander Gerlach, Alexander Hinderhofer, Christian Frank, Ute Heinemeyer, and Frank Schreiber — Institut fuer Angewandte Physik, Universitaet Tuebingen, Auf der Morgenstelle 10, 72076 Tuebingen Germany

The relation between optical and structural properties of organic semiconductors in thin films is crucial for their fundamental understanding as well as their application in electronic devices. Here we present first results of simultaneous in-situ real-time measurements of X-ray reflectivity (XRR) and differential reflectance spectroscopy (DRS) of perfluorinated copper phthalocyanine (F_{16}CuPc) thin films grown on SiO_2/Si wafers. Using DRS we determine the optical absorption spectra of the thin films starting from monolayer coverage whereas real-time XRR provides structural information about the film growth. After a rapid decrease of the reflectivity in the monolayer regime we observe intensity oscillations in time at constant qz with a strong damping. By calibrating film thickness d(t), we found oscillation period of 1.45 nm at 1/2q Bragg, which correspond to the lattice spacing of standing F_{16}CuPc molecules. This behaviour is characteristic for layer-growth with a finite roughness. In the monolayer regime the DRS signal shows a broad absorption peak at $\sim$2.0 eV, while for coverages of more than one monolayer an additional and relatively sharp peak appears at $\sim$1.6 eV. These results indicate that the film structure in the monolayer regime is different from the layer-growth regime.

DS 44.3 Fri 10:45 H8

In-situ Photoconduction Measurements of Mixed Films to Detect Isolated Clusters of Molecular Semiconductors — •Dominik Klaus, Christopher Keil, and Derck Schlettwein — Institute of Applied Physics, Justus-Liebig-University Giessen, Germany. email:schlettwein@uni-giessen.de

A cone-shaped subphthalocyanine (*SubPcBCl*) absorbing in the green was used as an electron donor and a planar perfluorinated phthalocyanine ($F_{16}PcCu$) absorbing in the red as an electron acceptor to discuss their applicability as a photosensitive material. Mixed thin films (60 nm) of increasing contents of *SubPcBCl* were studied that were prepared by physical vapour deposition on electrode structures on glass. Conduction measurements were performed under illumination at three distinct wavelengths across the visible range of the solar spectrum during growth and conditioning of the films. Photocurrents were observed that indicated the expected contributions to the net photoconduction of both molecules but also anomal, negative contributions were found, leading to a decreased conduction under illumination, showing the presence of isolated clusters for films rich in *SubPcBCl*. This behaviour indicates a light-induced trapping of electrons in insulating pockets under illumination with green and blue light.

DS 44.4 Fri 11:00 H8

Coupling effects in heterostructures of Pentacene and perfluorinated Pentacene studied by optical spectroscopy — •Katharina Broch[1], Ute Heinemeyer[1], Alexander Hinderhofer[1], Falk Anger[1,2], Oriol Ossó[2], Reinhard Scholz[3], Alexander Gerlach[1], and Frank Schreiber[1] — [1]Institut für Angewandte Physik, Auf der Morgenstelle 10, 72076 Tübingen — [2]MATGAS 2000 AIE, Campus de la UAB, 08193 Bellaterra — [3]Walter Schottky Institut, Technische Universität München, Am Coulombwall 3, 85748 Garching

Heterostructures of organic semiconductors gain increasing interest in the last years because of their potential applications in organic electronics. To optimize those devices the understanding of the intermolecular coupling is crucial. Therefore, we investigate the optical absorption spectra of heterostructures and possible differences to the spectra of their single components. The combination of pentacene (PEN) with perfluorinated pentacene (PFP) is promising due to their similar geometric structure which can give rise to coevaporated films with a significant level of intermixing and accordingly an efficient intermolecular coupling. Indeed, performing in-situ-measurements with differential reflectance spectroscopy and spectroscopic ellipsometry we find features in the absorption spectra of mixed films that cannot be explained by a linear combination of the single film spectra. In the energy range between 1.4 eV and 2.4 eV spectra of PFP and PEN single and coevaporated films with different mixing ratios are compared and possible theoretical scenarios for coupling effects are discussed.

DS 44.5 Fri 11:15 H8

In Situ Spectroscopic Investigation of CuPc Thin Films Grown on Vicinal Si(111) — •Li Ding, Marion Friedrich, Ovidiu Gordan, and Dietrich R. T. Zahn — Semiconductor Physics, Chemnitz University of Technology, D-09107 Chemnitz, Germany

Spectroscopic ellipsometry (SE) and reflection anisotropy spectroscopy (RAS) [1] are both surface sensitive and non-destructive techniques. SE is used to determine the dielectric functions, from which the out-of-plane anisotropy of thin films can be deduced. RAS is capable to measure the very tiny in-plane anisotropy in the order of 10^{-3}.

SE and RAS are employed simultaneously to monitor the growth process of Copper phthalocyanine (CuPc) thin films on passivated vicinal Si(111), in order to investigate the change in anisotropy and molecular orientation with increasing film thickness. The films were grown by organic molecular beam deposition (OMBD). The RAS features of CuPc are linearly dependent on the film thickness in the range of 30 nm, indicating a strong influence of the surface steps on the in-plane molecular alignment in the film. The in situ SE spectra are analyzed to investigate the change in the out-of-plane molecular orientation.

References

[1] P. Weightman, D. S. Martin, R. J. Cole, and T. Farrell, Rep. Prog. Phys. 68, 1251 (2005).

DS 44.6 Fri 11:30 H8

Model simulations of magneto-optical Kerr effect spectra of

organic films — •Klaus Seidel, Michael Fronk, Dietrich R. T. Zahn, and Georgeta Salvan — Physics Department, Chemnitz University of Technology, D-09107 Chemnitz, Germany

The rotation of the light polarization upon transmission through a magnetized sample is known as the Faraday effect, and the change in the ellipticity as magnetic circular dichroism (MCD). The change in the polarization state induced by reflection on a sample under magnetic field is known as magneto-optical Kerr effect (MOKE). These effects have their origin in the modification of the dielectric properties of the material in the presence of a magnetic field and can be described by a material parameter Q, the so-called Voigt constant, which occurs in the off-diagonal components of the macroscopic dielectric tensor. The MCD spectra are commonly simulated using the Faraday A, B, and C terms and compared to the experimental spectra in order to determine the number of the optical transitions, their energy position, and their electronic origin. In this work we apply the same approach to simulate the Voigt constant of Copper-Phthalocyanine films. In a second step we calculate, with the same set of parameters describing the optical transitions, the MOKE spectra and minimize the least square deviation from the experimental data.

DS 45: Organic Thin Films II

Time: Friday 12:00–13:00 Location: H8

DS 45.1 Fri 12:00 H8

OLEDs under high current densities — •Daniel Kasemann, Hartmuth Fröb, and Karl Leo — Institut für Angewandte Photophysik, Technische Universität Dresden, 01062 Dresden, Germany

Organic solid state lasers combine the flexibility of organic materials with the technological advantages of a solid state light emitter. Various optically pumped devices have been shown, comprising different resonator types like DFB and VCSEL design. Nevertheless, direct electrical pumping has not been achieved yet. The main obstacle here is the high excitation density needed in the active layer. The inversion is easily created by pulsed optical pumping, but additional losses prevent the excitation to reach the critical point when driven electrically.

To estimate the dimensions of the additional losses, we investigate full pin-OLEDs under high current densities and compare the behaviour of singlet and triplet emitter materials. The singlet emitter system uses Alq_3 doped by DCM as emitting layer. The triplet system is an efficient OLED based on α-NPD doped by $Ir(MDQ)_2(acac)$, a red phosphorescent emitter[1]. In pulsed operation, these devices sustain current densities in the range of kA/cm^2 without the need of additional cooling of the sample. To obtain an insight in the behaviour in this operation range, we compare power dependent emission spectra as well as electro-induced absorption (EIA) measurements at high current densities.

[1] R. Meerheim et al., J. Appl. Phys. **104**, 014510 (2008)

DS 45.2 Fri 12:15 H8

Use of Phthalocyanines as Photosensitizers for Dye-Sensitized Solar Cells Based on Zinc Oxide — •Melanie Rudolph[1], Jane Falgenhauer[1], Thomas Loewenstein[1], Nkosiphile Masilela[2], Mopelola Idowu[2], Tebello Nyokong[2], and Derck Schlettwein[1] — [1]Institute of Applied Physics, Justus-Liebig-University Giessen, Germany. email:schlettwein@uni-giessen.de — [2]Department of Chemistry, Rhodes University, Grahamstown, South Africa

Thin films of porous zinc oxide were prepared by electrodeposition from aqueous precursor solutions containing a structure- directing agent. Phthalocyanines (Pcs) with different central groups and different chemical substituents in the ligand were adsorbed onto the ZnO surface as photosensitizers. The obtained hybrid thin films were investigated with respect to their applicability in dye-sensitized solar cells. Aggregation is known to be a limiting factor for the solar energy conversion efficiency of sensitized semiconductor photoelectrodes, particularly in the case of phthalocyanines. The aggregation behaviour of the adsorbed Pc molecules was therefore analyzed by means of solid state UV/VIS transmission spectroscopy. Different methods were investigated to decrease intermolecular interactions within the photosensitizer layer. The photovoltaic performance of the dye-sensitized electrodes was analyzed by time-resolved photocurrent and photovoltage measurements as well as I(V) characteristics. These results were discussed in context with the aggregation tendency concluded from the UV/VIS data and the position of dye energy levels relative to the conduction band of ZnO.

DS 45.3 Fri 12:30 H8

Optimized light harvesting in thin film organic solar cells - modeling and experimental results — •André Merten, Uwe Dirks, Mauro Furno, Jan Meiss, Ronny Timmreck, Rico Schüppel, Karl Leo, and Moritz Riede — Institut für Angewandte Photophysik, Technische Universität Dresden

Optimal light absorption in the intrinsic layers of organic thin film solar cells is one of the basics for reaching high power conversion efficiencies.

However, multilayer interference phenomena have to be taken into account when designing the solar cell stack. Especially in the case of tandem solar cells, consisting of subcells with spectral complementary absorbers, interference effects have to be considered for current matching of the both subcells.

We present results of organic solar single and tandem solar cells, based on small molecules, which are designed and optimised by means of optical simulations based on a transfer-matrix-algorithm.

The optical simulation is verified by electrical characterization of solar cells with variation in layer thickness and by determining the spectral absorption by reflectance measurements with a fiber optical set-up, which also offers a validation of the layer deposition procedure at functional devices.

In addition to well controlled film thicknesses, the optical constants of the used organic materials are crucial for the optical simulation. Therefore, particular attention has to spend when determining theses constants and we present a sensitivity analysis for the predicted current densities with respect to errors in the optical constants.

DS 45.4 Fri 12:45 H8

Bulk-Carrier Analysis in OFETs Utilizing the True Channel Potential. — •Richa Sharma, Benedikt Gburek, Torsten Balster, and Veit Wagner — School of Engineering and Science, Jacobs University Bremen, Campus Ring 1, D-28759, Germany

In an Organic Field Effect Transistor (OFET), it is found that the electrical performance with respect to mobility and on-current increases with thickness. However, as the semiconductor thickness increases, the magnitude of the current in the off state is also found to increase deteriorating the on-off ratio. This is attributed to the increasing bulk current associated with increasing thickness. Therefore, it is crucial to understand the bulk behavior in OFETs at different operating regimes.

For this purpose, potential profiling of OFET channels of different thicknesses is done by 12 sense-fingers patterned in the channel of the transistor. The source, drain and the sense fingers are patterned in one step by optical lithography on the substrate. The semiconductor and insulator are spin-coated from solution and the top-gate is deposited through a shadow mask. The transfer curve measurements along with the potential measurements in the channel are done simultaneously. The corresponding potential profile for a particular gate voltage in the bulk regime is used to obtain the true potential in the channel. This channel potential along with the corresponding bulk current obtained from the transfer curve at different gate voltages is used to analyze the decrease of bulk conductivity in the off regime with increasing gate voltage. A proper model explains the experimental data by carrier depletion of the bulk with increasing gate voltage.

DS 46: Organic Thin Films III

Time: Friday 14:00–16:15 Location: H8

DS 46.1 Fri 14:00 H8

Role of the substrate in electronic structure, molecular orientation, and morphology of organic thin films: diindenoperylene on rutile TiO2(110) — •Maria Benedetta Casu, Britt-Elfriede Schuster, Indro Biswas, and Thomas Chassé — IPTC, University of Tübingen, Tübingen, Germany

Diindenoperylene (DIP, $C_{32}H_{16}$) is a perylene-based molecule that shows a very high hole mobility already in thin films, good film forming properties, and thermal stability. Sample preparation and photoemission experiments (X-ray photoelectron spectroscopy, XPS) were carried out in an ultrahigh vacuum system, The Ti 2p core level photoemission spectrum showed only a very weak low binding energy shoulder usually attributed to surface non-stoichiometry due to oxygen vacancies (3-5 % in our clean substrates). Atomic force microscopy (AFM) measurements were performed under ambient conditions in tapping mode. Near edge X-ray absorption spectroscopy (NEXAFS) measurements were performed at the beamline UE52-PGM at BESSY (Berlin). The results of our multitechnique investigation performed on diindenoperylene thin films deposited on rutile TiO_2(110) show island growth, with crystallites nucleating preferentially along the [1-10] substrate crystallographic axis. The findings evidence that the film properties at the interface are common to what found for a number of organic molecules deposited on the same substrate, revealing that the structural and morphological properties of organic thin films on rutile TiO_2(110) are essentially driven by its surface topography, with its rows of bridging oxygen atoms, while the molecular properties are less relevant.

DS 46.2 Fri 14:15 H8

Luminescence of PTCDA monolayers on NaCl in relation to their structural properties — •Mathias Müller, Eric Le Moal, Oliver Bauer, and Moritz Sokolowski — Institut für Physikalische u. Theoretische Chemie, Universität Bonn, Wegelerstraße 12, 53115 Bonn

On insulating surfaces the luminescence of monolayers of organic molecules can be studied in detail whereas on metals the luminescence is suppressed in most cases. The use of thin epitaxial NaCl(100) films grown on Ag(100) enabled us to perform spot profile analysis-LEED parallel to in-situ photoluminescence spectroscopy. Under optimized evaporation conditions we obtain different PTCDA monolayer structures, namely a commensurate 3x3 superstructure, an incommensurate herringbone-structure, and a disordered phase. All phases have interesting photoluminesce properties with sharp peaks and a well resolved vibronic finestructure in common. Besides, their luminescence spectra differ significantly in their energetic positions. Calculations based on a point-dipole model show that the corresponding exciton band structures have to be described by J-aggregates. This allows to explain the observed energetic differences of the luminescence spectra of these phases in detail. Funding by DFG research unit 557 is gratefully acknowledged.

DS 46.3 Fri 14:30 H8

Standing and lying α-6T molecules probed by PEEM spectroscopy — •Thorsten Wagner, Daniel Roman Fritz, Martin Oehzelt, and Peter Zeppenfeld — Johannes Kepler University Linz, Institute of Experimental Physics, Austria

The growth of α-sexithiophene (α-6T) depends strongly on the quality of the substrate surface: If the surface is clean and well ordered, the molecules are flat lying on the surface and form characteristic needles. If the surface is disordered, they grow in a upright standing manner forming platelet like crystallites [1]. We have applied photoelectron emission microscopy (PEEM) to study the growth of α-6T films on Ag(110) at different temperatures. By using a Hg-lamp with a photon energy of 4.9 eV it is not possible to overcome the ionization threshold of the molecule itself. Therefore, thick films of the molecules do not emit photoelectrons themselves but absorb these emitted from the metal substrate. Due to the coupling to the metallic substrate the first wetting layer shows an increased PEEM intensity. By applying high energy light sources available in the lab (D_2 with 6.4 eV and HeI with 21.2 eV) one can overcome the ionization potential and actually probe photoelectrons originating from the organic film. As the PEEM also allows energy filtering of the images, it is possible to probe the density of states on a 50 nm scale. The data reveal different emission spectra for the needles and the platelet like crystallites due to the orientation of the molecules in agreement with Duhn and Ivanco [1].

[1] S. Duhm *et al.*, Nature Materials **7**, 326 (2008) and J. Ivanco *et al.*, Surf. Sci. **601**, 178-187 (2007)

DS 46.4 Fri 14:45 H8

Energy level alignment at sexithiophene-fullerene heterojunctions from photoelectron spectroscopy: differentiating between intrinsic and extrinsic energy shifts — •Raphael Schlesinger[1], Hendrik Glowatzki[1], Johannes Frisch[1], Ralf-Peter Blum[1], Patrick Amsalem[1], Antje Vollmer[2], Jürgen P. Rabe[1], and Norbert Koch[1] — [1]Humboldt-Universität zu Berlin, Institut für Physik, 12489 Berlin, Germany — [2]HZB-Bessy II Albert-Einstein-Straße 15, 12489 Berlin, Germany

Ultraviolet photoelectron spectroscopy (UPS) was used to study the electronic structure of heterojunctions of sexithiophene (6T) and C_{60} on Au, Ag, and PEDT:PSS. Our results suggest that a monolayer of 6T on PEDT:PSS is lying flat, while molecules in multilayers stand vertically upright. The highest occupied molecular orbital (HOMO) of the 6T monolayer is less than 0.2 eV below the Fermi-level, while for multilayer 6T films the HOMO is pinned at 0.4 eV below the Fermi-level. This difference in binding energy of the frontier 6T levels is attributed to a charge-exchange reaction between 6T and PEDT:PSS, which is confined to the 6T monolayer only. The energy level alignment at the C_{60}/6T interface is found to follow the vacuum level alignment model. We will further highlight that effects often assigned to band bending in organic molecule films may well be induced by the UPS measurement itself. 6T films on PEDT:PSS exhibited a non-reversible shift of the energy levels/work function to higher binding energies by up to ca. 0.5 eV as a function of illumination with ultraviolet light (UV) that is commonly used to excite photoelectrons in UPS experiments.

DS 46.5 Fri 15:00 H8

Structural order of perfluoropentacene in fiber-textured and expitaxial films on amorphous and single crystalline substrates — •Ingo Salzmann[1], Martin Oehzelt[2], Steffen Duhm[1], Bernhard Wedl[3], Dmitrii Nabok[4], Jürgen P. Rabe[1], and Norbert Koch[1] — [1]Humboldt Universität zu Berlin, Germany — [2]Johannes Kepler Universität Linz, Austria — [3]Technische Universität Graz, Austria — [4]Montanuniversität Leoben, Austria

Synchrotron X-ray diffraction reciprocal space mapping (RSM) was performed on fiber-textured perfluoropentacene (PFP) thin films on SiO_x to determine the crystal structure of a monoclinic thin-film phase [1]. In a recent study, the growth of PFP on Ag(111) was investigated by X-ray standing waves and specular X-ray scattering reporting a flat adsorption geometry within the monolayer and a structural transition to an unknown (lying) herringbone structure upon subsequent growth [2]. We demonstrate an approach to solve unknown thin-film polymorphs on single crystalline substrates through a combination of RSM, X-ray diffraction pole figure technique (XRD-PF) and an appropriate variable substrate choice. Taking advantage of both the fiber-texture of Highly Ordered Pyrolytic Graphite (HOPG) and the low surface roughness we determined a structure solution of the triclinic polymorph of PFP/HOPG by RSM and proved the same to be present on Ag(111), Au(111) and Cu(111) by XRD-PF deriving the epitaxial relationships to the substrates.

[1] I. Salzmann et al., Langmuir, 24, 7294 (2008)

[2] S. Duhm et al., submitted.

DS 46.6 Fri 15:15 H8

template induced area selective growth: control over patterning of organic semiconductors — •Wenchong Wang, Dingyong Zhong, Chuan Du, Harald Fuchs, and Lifeng Chi — Physikalisches Institut and Center for Nanotechnology (CeNTech), Universität Münster, 48149 Münster, Germany

Functional small-molecular-weight organic molecules have received great scientific and technological interest due to their promising applications in electronics and optoelectronics. However, their future success in applications will strongly depend on the fabrication processes that include feasible methods for patterning. Here we present two strategies for area selective growth of organic molecules based on different mechanisms, namely binding-energy-difference-induced and step-edge-induced growth. Molecules may prefer to nucleate on material with which molecules have larger binding energy from other area when diffuse on pre-patterned substrate. Fully uniform nucleation control at the predefined locations can be achieved by an appropriate selection of the growth parameters and template dimensions. Molecules can also be controlled to nucleate at the edge of the template first, and grow laterally due to strong interaction such as π-π interaction of aromatic molecules, resulting in area selective growth of molecules on topographically low area of substrate. The technique can be used to grow crack-free, crystalline films with large domain sizes, presenting significantly increased charge mobility in comparison with un-patterned substrates. Further more, the two mechanisms can be combined together to separate molecules at defined locations.

DS 46.7 Fri 15:30 H8

Coverage and Morphology Dependence of Dip Coated Organic Films on Withdrawal Velocity — •Tomás Corrales[1,2], Pía Homm[2], Piero Ferrari[2], María J. Retamal[2], Edgardo A. Cisternas[3,2], Valeria del Campo[4,2], and Ulrich G. Volkmann[2] — [1]Max-Planck-Institut für Polymerforschung, Mainz, Germany — [2]Dept. of Physics, P. Universidad Católica de Chile, Santiago de Chile — [3]Dept. of Research and Development, Tecnología Integral S.A., Santiago de Chile — [4]Dept. of Hydraulic and Environmental Engineering, P. Universidad Católica de Chile, Santiago de Chile

In this work we dip-coat *n*-dotriacontane onto silicon substrates, coated with their native oxide film ($\approx$15 Å), from an *n*-heptane solution varying systematically the withdrawal velocity from 0.04 cm/min to 9.25 cm/min. After coating, we study the resulting films with AFM and SEM. We observe the formation of self-assembled monolayer structures with different coverage and morphologies, depending on the withdrawal velocity: For a pulling velocity of 1 cm/min we observe a minimum coverage of $\approx$11% while a maximum coverage of $\approx$54% is reached for the slowest velocity (0.04 cm/min). For velocities higher than 5 cm/min we observe a stabilization at a coverage of $\approx$35%. We relate this behavior to the transition from a gravity driven film growth to an entrained film regime, proposed by M. Ghosh et al. [1]. We also find that the morphology of these structures depends strongly on the withdrawal velocity.

[1] M. Ghosh, F. Fan, K.J. Stebe, Langmuir 23 (4), 2007.

This work is supported by FONDECYT 1060628.

DS 46.8 Fri 15:45 H8

Thin films of new organic charge transfer systems — •Milan Rudloff and Michael Huth — Physikalisches Institut, Max-von-Laue-Str. 1, D-60438 Frankfurt am Main

We deal with the preparation and characterization of thin films of organic charge transfer (CT) systems. These systems are made of donor and acceptor molecules that exhibit an additional electrostatic attraction due to Coulomb interaction between donor and acceptor. The electronic properties of the resulting new compound (depending on crystal structure, temperature and pressure) can be those of an insulator, a semiconductor, a metal or a superconductor.

The thin films are prepared by organic molecular beam deposition (OMBD). The OMBD process takes place inside an UHV chamber in which the source materials are (co-) sublimed and deposited onto a substrate. After that the samples are characterized by light and atomic force microscopy, X-ray diffractometry and (temperature dependent) transport measurements.

Our work focuses on new donor-acceptor combinations with the aim to prepare CT compounds that are yet unknown. The results presented here relate to experiments with some of these new donor(D)-acceptor(A) pairs, e.g. tetramethoxypyrene (D) + tetracyanoquinodimethane (A) and tetrathiafulvalene (D) + tetraketopyrene (A).

DS 46.9 Fri 16:00 H8

Direct Write 3-Dimensional Nanopatterning using Probes — •Felix Holzner[1], Armin Knoll[1], David Pires[1], Ute Drechsler[1], Michel Despont[1], Heiko Wolf[1], James Hedrick[2], Anuja DeSilva[3], and Urs Duerig[1] — [1]IBM Research - Zurich, Switzerland — [2]IBM Research - Almaden, USA — [3]IBM Research - Watson, USA

A high-resolution probe based patterning method is presented using organic resists, that respond to the presence of a hot tip by local material desorption. Thereby arbitrarily shaped patterns can be written in the organic films in the form of a topographic relief. Line gratings with a half-pitch of 15 nm have been fabricated.

Moreover, three dimensional patterns can be written by controlling the amount of material removal. The patterns can be readily transferred into silicon using standard RIE technology. The new technique offers a cost-effective and competitive alternative to high-resolution electron-beam lithography in terms of both resolution and speed.

DS 47: [O] Plasmonics and Nanooptics VII (Joint Session DS/O/HL)

Time: Friday 11:15–13:00 Location: H32

DS 47.1 Fri 11:15 H32

Metamaterial sensor for glucose and molecular monolayers using the plasmonic analog of EIT — •Martin Mesch[1], Na Liu[1], Thomas Weiss[1], Carsten Sönnichsen[2], and Harald Giessen[1] — [1]4th Physics Institute, University of Stuttgart, Germany — [2]Institute of Physical Chemistry, University of Mainz, Germany

We utilize the plasmonic analog[1] of electromagnetically induced transparency (EIT) to construct an optical LSPR (localized surface plasmon resonance) sensor. A combination of stacked gold dipole and quadrupole antennas exhibits a sharp spectral resonance, which shifts for changes in the structures' dielectric environment. To characterize the sensor, aqueous glucose solutions with concentrations between 0% and 25% have been measured in a custom flow cell by Fourier transform infrared spectroscopy. The results reveal a sensitivity of 374 nm per refractive index unit, corresponding to a figure of merit (sensitivity/linewidth) of 4.1. We compare our measurements to S-matrix simulations and give a recipe to determine the most sensitive structure geometry. To our knowledge, this is up to date the most sensitive lithographically manufactured LSPR sensor design. Additional experiments demonstrate the ability to detect a single molecular layer of biotin/streptavidin. [1] N. Liu et al., Nature Materials 8, 758 (2009)

DS 47.2 Fri 11:30 H32

Optical properties of a metallic meander Fabry-Perot cavity — •Liwei Fu[1], Heinz Schweizer[1], Thomas Weiss[2], Harald Giessen[1], Philipp Schau[3], Karsten Frenner[3], Steffen Maisch[3], and Wolfgang Osten[3] — [1]4th Physics Institute, University of Stuttgart, Pfaffenwaldring 57, 70550 Stuttgart, Germany — [2]LASMEA, Université Blaise Pascal, F-63177 Aubière Cedex, France — [3]Institut für Technische Optik, University of Stuttgart, Pfaffenwaldring 9, 70550 Stuttgart, Germany

A single layer metallic meander structure is favorable to couple photons with surface plasmon polaritons and, as a result, a resonant enhanced transmission can be observed. A combination of two single-meander layers forms a Fabry-Perot cavity with frequency selective mirrors. In this contribution we investigate its optical properties. At the proper distance, the cavity behaves as a single layer meander, in which enhanced transmission and negative mode dispersion are present. In contrast to the single layer, however, the surface waves from the two mirrors are still coupled together, resulting in an amplified longitudinal E-field propagating backwards inside the cavity. The backward wave can be observed at visible frequencies with low loss and high transmittance for structural parameters that are well suited for nanofabrication. Such a compact realization of negative refraction is a promising approach for applications of subwavelength imaging, polarization beam splitting, and delay line approaches.

DS 47.3 Fri 11:45 H32

Dynamical response of split-ring molecules for metamaterials — •Stephan Bernadotte[1,2,3], Wim Klopper[1,2], and Ferdinand Evers[1,3] — [1]Institut für Nanotechnologie, Karlsruher Institut für Technologie — [2]Lehrstuhl für Theoretische Chemie, Institut für Physikalische Chemie, Karlsruher Institut für Technologie — [3]Institut für Theorie der Kondensierten Materie, Karlsruher Institut für Technologie

We investigate the dynamical properties of molecular crystals (matrices) built up from nanometer sized ring shaped, conjugated molecules, which are candidate systems for negative index materials with frequencies in the optical regime. The response properties of such materials near their dynamical resonances can be understood in terms of an LRC circuit. In the conventional modeling of metamaterials, the circuit parameters enter (essentially) as phenomenological quantities. By contrast, in the present work they will be calculated from a microscopic tight binding model of a molecular Hamiltonian employing the Kubo approach.

We find that the LRC resonances of the molecular structures correspond to plasmonic excitations. By comparing to an analytical calculation, we can study in which way the plasmon resonances (and residues) depend on the molecule's electronic structure. On a qualitative level, our study also includes an investigation of the sensitivity of the dynamical response to the damping of the plasmons. Finally, we analyze the impact of cross-talk among the molecules within the matrix and the importance of birefringence terms.

DS 47.4 Fri 12:00 H32

Negative refraction in natural ferromagnetic metals — •Sebastian Engelbrecht, Alexey Shuvaev, and Andrei Pimenov — Experimentelle Physik 4, Universität Würzburg

It is generally believed that nature does not provide materials which show negative refraction. Up to now, the experiments with negative refraction have been realized with metamaterials or photonic crystals. As has been suggested recently, negative refraction in natural materials can be realized in ferromagnetic metals. Close to the ferromagnetic resonance (FMR) the real part of the magnetic permeability can reach negative values. This may lead to negative refraction as long as the dielectric permittivity is dominated by metallic response. This talk will provide experimental data of ferromagnetic metals (Fe,Co) which indeed show a range of negative refraction close to FMR in millimeter frequency range. In these materials the negative refractive index can be achieved even at room temperature.

DS 47.5 Fri 12:15 H32

Bragg Plasmonics — •Richard Taubert, Ralf Ameling, Lutz Langguth, Daniel Drégely, and Harald Giessen — University of Stuttgart, Germany

The investigation of plasmon-plasmon coupling has focused on near-field coupling until now. Only little work has been done on far-field interaction in plasmonic structures. We investigate a so-called 3D plasmonic crystal: four layers of nanowires are stacked in Bragg fashion, where the vertical distance matches half the resonance wavelength of the individual nanowire particle plasmon. The resonant far field coupling leads to the formation of a plasmonic band gap spanning almost one octave.

The structure was fabricated using layer-by-layer stacking. We investigate the dependence of the optical spectra on layer number and distance tuning. Scattering matrix calculations agree very well with our experimental findings.

DS 47.6 Fri 12:30 H32

Al nanostructures for metamaterials in visible region and biosensing — •Shankar K. Jha[1], Yogesh Jeyaram[1], Mario Agio[2], Jörg F. Löffler[1], and Yasin Ekinci[1,3] — [1]Laboratory of Metal Physics and Technology, ETH Zurich, 8093 Zurich, Switzerland — [2]Laboratory of Physical Chemistry, ETH Zurich, 8093 Zurich, Switzerland — [3]Paul Scherrer Institute, 5232 Villigen-PSI, Switzerland

Metamaterials are artificially engineered materials having electromagnetic material properties that are not readily found in nature. Owing to their potential applications like sub-wavelength imaging, negative refractive index, optical cloaking etc., these materials have been extensively studied in the microwave and optical regimes including in red wavelengths. We report development of metamaterials down to blue range. We studied optical properties of two-dimensional arrays of aluminum nanosandwiches. Strong magnetic response and negative permeability are observed down to 400 nm wavelength, paving the way towards metamaterials operating in the visible range. In addition we discuss the superior performance of such structures in biosensing.

DS 47.7 Fri 12:45 H32

Electromagnetic polarisation twisting mediated by plasmon / nanostructure interaction — •Brian Ashall[1], Brian Vohnsen[1], Stephan Schwieger[2], Erich Runge[2], Michael Berndt[3], and Dominic Zerulla[1] — [1]School of Physics, University College Dublin, Dublin 4, Ireland. — [2]Theoretical Physics I, Technische Universität Ilmenau, 98684 Ilmenau, Germany. — [3]Max Planck Institute of Molecular Cell Biology and Genetics, 01307 Dresden, Germany.

The design and architecture of nanostructures for the purpose of controlling and manipulating Surface Plasmon Polariton (SPP) dynamics is currently a focal point of research. Here, we present the first instance of plasmon mediated polarisation reorientation observed in the farfield with no associated reemission directional change [1]. Specifically, it is demonstrated that, as a result of the interaction between SPPs and tailor designed nanostructures of 3-fold symmetry characteristics [2], a polarisation twisting of the SPP mediated reradiated light is attained. It is shown that the dynamics of such an interaction can be controlled externally, enabling active control of the out-going polarisation orientation. In order to further understand the origin of the processes involved, Green's function based simulations of the interactions are presented and confirm that the origin of the polarisation twisting can be explained via asymmetrical in-plane SPP scattering.

[1] B. Ashall, B. Vohnsen, M. Berndt, D. Zerulla; Phys. Rev. B, 80(20) (2009)

[2] B. Ashall, M. Berndt, D. Zerulla; Appl. Phys. Lett. 91(20), 203109 (2007)

DS 48: [O] Organic Electronics and Photovoltaics III (Joint Session DS/CPP/HL/O)

Time: Friday 11:15–12:45 Location: H40

DS 48.1 Fri 11:15 H40

WO3 under, in and on CuPc - A doping mechanism for organic semiconductors — •Corinna Hein, Eric Mankel, Thomas Mayer, and Wolfram Jaegermann — TU Darmstadt, FG Oberflächenforschung, Petersenstraße 32, 64287 Darmstadt

Doping of organic semiconductors plays an important role for the development of organic devices like photovoltaic cells or organic light emitting diodes. P-doping of CuPc which is frequently used as hole conductor was performed successfully by coevaporation of the CuPc matrix and the WO3 dopant showing good doping efficiency and limit. The Fermi level determined by synchrotron induced photoemission shifts gradually with the concentration of dopant up to 690meV. To clarify the doping mechanism band alignment of both CuPc/WO3 and WO3/CuPc interfaces was determined. The work function difference of the two materials is overcome by band bending and an interface dipole. The dipole is 2eV for CuPc/WO3 and 1.4eV for WO3/CuPc lowering the amount of transferred charge and therefore limiting the doping efficiency. The sum of band bending at the interface adds up to 0.5eV for the CuPc/WO3 interface and 1.1eV for CuPc deposited on WO3. The Fermi level shift in the composites fits to this range in accord to a doping model assuming cluster growth of WO3 within CuPc. The model could be directly proofed by transmission electron microscopy distinguishing the two phases of CuPc and WO3 with a cluster size of approximately 5nm.

DS 48.2 Fri 11:30 H40

Mixed Self-Assembled Monolayers on Au(111): Understanding the Level Alignment and Work-Function Modification. — •Ferdinand Rissner[1], David A. Egger[1], Lorenz Romaner[2], Georg Heimel[3], and Egbert Zojer[1] — [1]Institute of Solid State Physics, Graz University of Technology, Austria — [2]Chair of Atomistic Modelling and Design of Materials, University of Leoben, Austria — [3]Institut für Physik, Humboldt-Universität zu Berlin, Germany

In organic electronics, coverage of electrodes with appropriate self-assembled monolayers (SAMs) is a well-known technique for enhancing the performance of devices; by modification of the electrode work function, Φ, charge-carrier injection barriers can be optimized. Mixing molecules which show a work-function increasing effect ($\Delta\Phi > 0$) with molecules decreasing Φ was experimentally found to allow for tuning of Φ over a wide range (as a function of the mixing ratio). [1]

For "pure" SAMs of π-conjugated oligophenylene derivatives, the mechanisms controlling the metal/SAM interface energetics have been extensively investigated over the past years. Here, we present density-functional theory based slab-type band structure calculations on the energetics of mixed monolayers. We find and explain significant differences in the energy-level alignment compared to what is known from the respective pure layers.

[1] K.-Y. Wu, S.-Y. Yu and Y.-T. Tao, Langmuir, **2009**, 25 (11), pp 6232-6238.

DS 48.3 Fri 11:45 H40

Analysis of systematic heat treatment of TiO2 nanocrystalline films for solid-state dye sensitized solar cells using photoelectron spectroscopy — •Xianjin Feng, René Hock, Eric Mankel, Thomas Mayer, and Wolfram Jaegermann — Institute of Materials Science, Darmstadt UniVersity of Technology, D-64287 Darmstadt, Germany

In this contribution we investigated the effect of heat treatment on the chemical and electronic structures of TiO2 nanocrystalline films for solid-state dye sensitized solar cells (SDSC). The samples were heated in air by an air-gun and a hot plate, respectively, within the temperature range of 300-600°C. The samples were chemically and electronically characterized using synchrotron-induced photoelectron spectroscopy (SXPS) and X-ray photoemission spectroscopy (XPS). The most prominent chemical variation after heating by air-gun was found in the SXPS the intensity increase of the Na2p core level and obvious changes both in the O2s core level and O2p valence band were also observed at 450°C. An increase in the Na1s core level was also observed in the XPS study. For the heat treatment using a hot plate, the intensity of the Na2p core level increased less strongly and no obvious change in the O2s core level and O2p valence band was observed even at 600°C. In both cases of heat treatment, the oxygen vacancies VO-related gap states around 1.3 eV and states just below the Fermi level were observed in the gap region and the intensity of the VO-related gap states decreased obviously after heating and almost vanished at high temperatures.

DS 48.4 Fri 12:00 H40

Vanadyle and perfluoro vanadyle phthalocyanine on gold: unseen metastable modification and interfacial reaction — •Indro Biswas, Heiko Peisert, and Thomas Chassé — Institut f. Physikalische u. Theoretische Chemie, Universität Tübingen, Auf der Morgenstelle 8, 72076 Tübingen

Vanadyle phthalocyanine (PcVO) and perfluorinated-vanadyle phthalocyanine (F$_{16}$PcVO) are of the same inside-out-umbrella structure as the extensively investigated titanyle phthalocyanine. Just in the recent years, interest on these molecules has grown again. They exhibit some very surprising properties. Thin films of PcVO and F$_{16}$PcVO on polycrystalline gold have been examined using photoemission, X-ray absorption, optical spectroscopy, and Kelvin probe measurements. In addition to surprisingly good self-ordering abilities of both materials, an interface reaction including the fluorine substituents in F$_{16}$PcVO has been observed, and the application of the minimal invasive Kelvin probe method allowed the investigation of the undisturbed metastable Phase I of PcVO with a different interface formation, which will be transformed by conventional spectroscopic methods.

1 C. H. Griffiths, M. S. Walker, P. Goldstein, *Polymorphism in Vanadyle Phthalocyanine*, Mol. Cryst. Liq. Cryst. 33 (1976) 149.

DS 48.5 Fri 12:15 H40

Photoemission spectroscopy investigations of silicon organic dye interfaces for photovoltaic applications — •Andreas Decker[1], Thomas Mayer[1], Wolfram Jaegermann[1], Sabin Suraru[2], and Frank Würthner[2] — [1]Fachgebiet Oberflächenforschung, Fachbereich Materialwissenschaften, Technische Universität Darmstadt — [2]Institut für Organische Chemie, Universität Würzburg

In a new solar cell concept, organic dyes (small molecules) are embedded in the hydrogenated microcrystalline i-layer of a silicon p-i-n structure to enhance the optical absorption. This approach aims at an increase in efficiency and a decreased silicon absorber layer thickness, thus potentially lowering deposition time and production cost.

The electrical lineup of the dye orbitals versus the silicon band edges plays a vital role for this sensitization process because a driving force is needed for the transfer of photogenerated electrons and holes from the dye molecules to the silicon matrix. For the two dyes Cl$_4$MePTCDI and CuPc the electrical lineup on our model substrate, hydrogen terminated n-type Si(111), was investigated with photoemission interface experiments. Si(111):H was prepared from wafers with a native oxide by two-step wet-chemical etching in NH$_4$F which leads to clean and flat terraces as shown in AFM measurements. By comparison of calculations with XPS measurements the Si(111):H surface was found to have flat bands, i. e. showing no Fermi level pinning due to dangling bonds or fresh adsorbates originating from the sample transport through air to the UHV system, thus being a suitable substrate for interface experiments.

DS 48.6 Fri 12:30 H40

Band alignment studies of ZnO-ZnS-CIS interfaces — •Carsten Lehmann, Andreas Hofmann, Alexandra Dombrowa, and Christian Pettenkofer — Helmholz-Zentrum Berlin, Berlin, Deutschland

With respect to thin film solar cells based on CuInS$_2$ and ZnO ZnS is a promising alternative to CdS as buffer layer material [1,2]. A MOMBE process based on diethylzinc and water is investigated on CuInS$_2$(112) thin films. A ZnS buffer layer grows epitaxially using the surplus of sulfur in the eventually present CuS$_x$ layer. A ZnO film grows on top of the .8 nm thick ZnS layer with its own lattice parameters in (0001) direction. Step-by-step analysis of this ZnO-ZnS-CIS interface yielded a band alignment favorable for photovoltaic applications [2]. We present in-situ preparation and step-by-step investigation on ZnO-ZnS-CIS interfaces with varying CIS substrates. CuInS$_2$(001) samples were prepared on GaAs(100) by gas source MBE (GSMBE) using TBDS as sulfur precursor. Sulfurization of CuIn films prepared by MBE and sputtering yielded polycrystalline CuInS$_2$ samples of 100nm up to 2.5μm thickness. The samples were investigated by XPS, UPS and LEED. We will discuss the interfaces with respect to the derived band aligments and their morphology. Furthermore we will compare the results to those of analogous experiments on CuInSe$_2$(112). [1] M. Bär, et. al., Journal of Applied Physics 99 (2006) [2] S. Andres, et. al., Thin Solid Films 518 (2009)