Thin Films Division
Fachverband Dünne Schichten (DS)

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Overview of Invited Talks and Sessions

(lecture rooms H 2013 and H 2032; Poster A - Galerie 2.OG)

Invited Talks

DS 1.1	Mon	9:30–10:00	H 2013	**Organic Spintronics five years later** — •Carlo Taliani
DS 1.2	Mon	10:00–10:30	H 2013	**Organic spintronics: can theory play a role?** — •Stefano Sanvito
DS 1.3	Mon	10:30–11:00	H 2013	**Spintronic and electro-mechanical effects in single-molecule transistors** — •Maarten R. Wegewijs
DS 2.1	Mon	11:45–12:15	H 2013	**Tunable electron spin resonance spectroscopy of multi-center paramagnetic molecular complexes in strong magnetic fields** — •Vladislav Kataev
DS 2.2	Mon	12:15–12:45	H 2013	**Coordinated metal centers: Single-molecule magnets and highspin to lowspin switching** — •Paul Müller
DS 2.3	Mon	12:45–13:15	H 2013	**Substrate-induced magnetic ordering and switching of iron porphyrin molecules** — •H. Wende, M. Bernien, J. Luo, C. Weis, N. Ponpandian, J. Kurde, J. Miguel, M. Piantek, X. Xu, Ph. Eckhold, W. Kuch, K. Baberschke, P. Srivastava, P.M. Panchmatia, B. Sanyal, P.M. Oppeneer, O. Eriksson
DS 6.1	Mon	9:30–10:15	H 2032	**High Speed Nano-Photonics** — •Gadi Eisenstein
DS 7.1	Mon	11:15–12:00	H 2032	**Recent advances of VCSEL photonics** — •Fumio Koyama
DS 7.4	Mon	12:30–13:00	H 2032	**Recent Advances on Long Wavelength VCSELs (> 1300 nm)** — •Markus C. Amann
DS 8.1	Mon	14:00–14:45	H 2032	**High Efficiency Nonpolar InGaN/GaN based Blue Light Emitting Diodes and Laser Diodes** — •Steven P. DenBaars, Mathew C. Schmidt, Robert Farrell, Daniel Fezzell, Stacia Keller, James S. Speck, Shuji Nakamura
DS 8.2	Mon	14:45–15:15	H 2032	**Polarization induced effects in GaN-based devices** — •Oliver Ambacher
DS 8.3	Mon	15:15–15:45	H 2032	**The optoelectronic chameleon - GaN-based light emitters from the UV to green** — •Michael Kneissl
DS 9.1	Mon	16:00–16:30	H 2032	**GaN-Photonics on Silicon** — •Alois Krost
DS 10.1	Mon	17:30–18:00	H 2032	**Nanotechnology based single-mode lasers for telecommunication and sensing** — Martin Kamp, Sven Höfling, •Alfred Forchel
DS 13.1	Tue	9:30–10:15	H 2032	**Film Production Technologies** — •Hans K. Pulker
DS 13.2	Tue	10:15–10:45	H 2032	**Innovative stationary and in-line sputter technologies for precision optical coatings** — •Peter Frach, Hagen Bartzsch, Joern-Steffen Liebig, Joern Weber, Volker Kirchhoff
DS 13.3	Tue	10:45–11:15	H 2032	**Novel Process Concepts for Ion Beam Sputtering Deposition** — •Kai Starke, Henrik Ehlers, Marc Lappschies, Nils Beermann, Detlev Ristau
DS 14.1	Tue	12:00–12:30	H 2032	**Demands on Coating Technologies in the Optical Component Industry** — •Marcus Serwazi
DS 14.2	Tue	12:30–13:00	H 2032	**Optische Prüfverfahren für die Qualitätssicherung in der Schicht- und Oberflächentechnik** — •Uwe Beck

DS 14.3	Tue	13:00–13:30	H 2032	**Mixed oxide coatings for advanced fs-laser applications** — •Marco Jupe, Marc Lappschies, Kai Starke, Detlev Ristau, Andrius Melninkaitis, Valdas Sirutkaitis, Igor Cravetchi, Wolfgang Rudolph
DS 15.1	Tue	14:30–15:00	H 2032	**The truth about ferromagnetic ZnO** — •Kay Potzger, Shengqiang Zhou, Georg Talut, Karsten Kuepper, Helfried Reuther, Arndt Mücklich, Jörg Grenzer, Manfred Helm, Jürgen Fassbender, Heidemarie Schmidt, Quingyu Xu, Michael Lorenz
DS 15.2	Tue	15:00–15:30	H 2032	**ZnO-based Hetero- and Quantum Well Structures for Light-Emitting Applications** — •Fritz Henneberger, Sergey Sadofev
DS 15.3	Tue	15:30–16:00	H 2032	**Large Area Deposition of Transparent Conductive Oxide Films** — •Bernd Szyszka, Volker Sittinger, Andreas Pflug, Stephan Ulrich, Felix Horstmann
DS 16.1	Tue	17:00–17:30	H 2032	**Zinc Oxide Nanostructures: Optical resonators and lasing** — •Klaus Thonke, Anton Reiser, Martin Schirra, Martin Feneberg, Guenther M. Prinz, Tobias Röder, Rolf Sauer, Johannes Fallert, Felix Stelzl, Heinz Kalt, Stefan Gsell, Matthias Schreck, Bernd Stritzker
DS 16.4	Tue	18:00–18:30	H 2032	**Electrochromic coatings and windows** — •Sabine Heusing
DS 16.5	Tue	18:30–19:00	H 2032	**Semiconducting metal oxides for gas sensors** — •Tilman Sauerwald, Thorsten Wagner
DS 19.1	Wed	14:30–15:00	H 2013	**Organometallic Nanojunctions Probed by Different Chemistries: Thermo-, Photo, and Mechanochemistry** — •I. Stich, M. Konopka, R. Turansky, J. Reichert, N. L. Doltsinis, H. Fuchs, D. Marx
DS 20.1	Wed	17:45–18:15	H 2013	**Designing the nanostructure of the organic polymer - metal interface** — •Stephan V. Roth
DS 21.1	Wed	14:30–15:00	H 2032	**Challenges and Chances with new materials in semiconductor device applications** — •Stefan Jakschik, Karl-Heinz Küsters
DS 21.2	Wed	15:00–15:30	H 2032	**Are Optical Measurements Sensitive to Quantum Confinement?** — •Alain Diebold
DS 22.1	Wed	16:45–17:15	H 2032	**Development of novel processes for atomic layer deposition of high-k dielectrics** — •Jaakko Niinistö, Kaupo Kukli, Mikko Ritala, Markku Leskelä
DS 22.2	Wed	17:15–17:45	H 2032	**Towards a better understanding of the dielectric collapse in high-K BST thin film capacitors** — •Regina Dittmann, Rafael Plonka, Nikolay Pertsev, Susanne Hoffmann-Eifert, Rainer Waser
DS 24.1	Thu	9:30–10:00	H 2013	**Nanostructures produced with energetic heavy ion projectiles** — •Christina Trautmann
DS 24.2	Thu	10:00–10:30	H 2013	**Low energy maskless implantation with high lateral resolution.** — •Jan Meijer, Sebastien Pezzagna, Dirk Reuter, Ivo W. Rangelow, Hartmut Wiggers, Fedor Jelezko, Inam Mirza, Jörg Wrachtrup, Ferdinand Schmidt-Kaler, Wolfgang Schnitzer, Kilian Singer
DS 24.3	Thu	10:30–11:00	H 2013	**Cluster ion-surface interactions: from meV to MeV energies** — •Kai Nordlund, Kristoffer Meinander, Tommi T. Järvi, Jarkko Peltola, Juha Samela
DS 26.1	Thu	13:45–14:15	H 2013	**Profiling of Fibre Texture Gradients by Anomalous X-ray Diffraction** — •M. Birkholz, N. Darowski, I. Zizak
DS 27.1	Thu	14:30–15:00	H 2013	**Surface engineering with ion beams: from self-organzied nanostructures to ultra-smooth surfaces** — •Frank Frost, Bashkim Ziberi, Axel Schindler, Bernd Rauschenbach
DS 27.2	Thu	15:00–15:30	H 2013	**Rare earth doping of GaN** — •André Vantomme
DS 27.3	Thu	15:30–16:00	H 2013	**Junction and Channel Engineering for Advanced Microprocessors** — •Manfred Horstmann
DS 35.1	Thu	17:00–17:30	H 2032	**Nanostructure and transport in regioregular polythiophenes and their block copolymers** — Rui Zhang, Bo Li, Jessica R. Cooper, Mihaela Iovu, Genevevie Sauve, David N. Lambeth, Detlef-M. Smilgies, Richard D. McCullough, •Tomasz Kowalewski
DS 36.1	Fri	10:15–10:45	H 2013	**Infrared ellipsometry on functional films at the solid-liquid-interface** — •Karsten Hinrichs
DS 36.2	Fri	10:45–11:15	H 2013	**Surface enhanced infrared spectroscopy** — •Annemarie Pucci
DS 37.1	Fri	13:30–14:00	H 2013	**Ambient pressure spectroscopy of catalytically active nanostructures: Mind the gap!** — •Günther Rupprechter

DS 37.2	Fri	14:00–14:30	H 2013	**Near-field Infrared Nanoscopy and Nanospectroscopy** — •Rainer Hillenbrand
DS 38.1	Fri	15:15–15:45	H 2013	**Vibrational dynamics on the nanoscale** — •Markus Raschke
DS 38.2	Fri	15:45–16:15	H 2013	**UHV-based TERS on adsorbed molecules** — •Bruno Pettinger, Jens Steidtner
DS 38.3	Fri	16:15–16:45	H 2013	**Tip enhanced Raman scattering on biological samples** — •Volker Deckert
DS 39.1	Fri	10:15–10:45	H 2032	**Vortex Manipulation in Superconductor/Ferromagnet Hybrid Nanosystems(*)** — •Victor Moshchalkov
DS 39.2	Fri	10:45–11:15	H 2032	**Investigating the interaction between single-crystalline antiferromagnetic films and ferromagnets** — •Wolfgang Kuch
DS 40.1	Fri	12:15–12:45	H 2032	**Influence of antiferromagnetic layers on the magnetization dynamics of exchange coupled thin films** — •Jeffrey McCord
DS 40.4	Fri	13:15–13:45	H 2032	**Ion Beam Induced Magnetic Nanostructures** — •Peter Varga

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VA 6.1	Wed	13:30–14:15	HE 101	**Structure formation, kinetics and mechanics in thin films and solids: from nanoscale to macroscopic properties in experiments and simulations.** — •S. G. Mayr

Invited talks of the joint symposium SYSA

SYSA 1.1	Tue	9:30–10:00	H 0105	**Level alignment at metal/organic interfaces** — •Fernando Flores
SYSA 2.1	Tue	10:45–11:15	H 0105	**Organic film growth and organic-metal interfaces** — •Norbert Koch
SYSA 2.5	Tue	12:00–12:30	H 0105	**Molecular n-doping of organic semiconductors** — •Antoine Kahn, Calvin Chan
SYSA 3.1	Tue	14:30–15:00	H 2013	**Charge transport and contact effects in organic semiconductors** — •Alberto Salleo, Leslie Jimison, Jonathan Rivnay, Ludwig Goris, Michael Toney
SYSA 4.1	Tue	16:30–17:00	H 2013	**Polymer electronics - Charge transport at organic-organic heterointerfaces** — •Henning Sirringhaus
SYSA 6.1	Wed	14:30–15:00	H 2013	**Organometallic Nanojunctions Probed by Different Chemistries: Thermo-, Photo, and Mechanochemistry** — •I. Stich, M. Konopka, R. Turansky, J. Reichert, N. L. Doltsinis, H. Fuchs, D. Marx
SYSA 7.1	Wed	17:45–18:15	H 2013	**Designing the nanostructure of the organic polymer - metal interface** — •Stephan V. Roth
SYSA 8.1	Thu	17:00–17:30	H 2032	**Nanostructure and transport in regioregular polythiophenes and their block copolymers** — Rui Zhang, Bo Li, Jessica R. Cooper, Mihaela Iovu, Genevevie Sauve, David N. Lambeth, Detlef-M. Smilgies, Richard D. McCullough, •Tomasz Kowalewski

Invited talks of the joint symposium SYNF

SYNF 2.1	Tue	14:30–15:00	A 151	**Tunable two-dimensional electron gases in correlated electronic systems** — •J. Mannhart, G. Hammerl, T. Kopp, C. Richter, C.W. Schneider, S. Thiel, N. Reyren, A.D. Caviglia, S. Gariglio, D. Jaccard, J.-M. Triscone, L. Fitting-Kourkoutis, D. Muller, C. Cheng, J. Levy
SYNF 2.2	Tue	15:00–15:30	A 151	**New physics from electron correlations at oxide interfaces** — •Warren E. Pickett, Rossitza Pentcheva
SYNF 2.3	Tue	15:30–16:00	A 151	**Gigantic magnetoelectic responses in hellimagnets** — •Y. Tokura
SYNF 2.4	Tue	16:00–16:30	A 151	**Electrical field control of ferromagnets using multiferroics** — •Ramamoorthy Ramesh
SYNF 2.5	Tue	16:30–17:00	A 151	**Spintronics with multiferroic materials** — •Agnes Barthelemy
SYNF 2.6	Tue	17:00–17:30	A 151	**Magnetoelectric effects at multiferroic interfaces** — •Evgeny Tsymbal

Sessions

DS 1.1–1.5	Mon	9:30–11:30	H 2013	**Towards Molecular Spintronics**
DS 2.1–2.5	Mon	11:45–13:45	H 2013	**Towards Molecular Spintronics**
DS 3.1–3.6	Mon	14:30–16:00	H 2013	**Organic Thin Films**
DS 4.1–4.5	Mon	16:15–17:30	H 2013	**Organic Thin Films**
DS 5.1–5.6	Mon	17:45–19:15	H 2013	**Organic Thin Films**
DS 6.1–6.4	Mon	9:30–11:00	H 2032	**Semiconductor Nanophotonics: Materials, Models, Devices - High Speed Photonics**
DS 7.1–7.4	Mon	11:15–13:00	H 2032	**Semiconductor Nanophotonics: Materials, Models, Devices - Surface Emitters**
DS 8.1–8.3	Mon	14:00–15:45	H 2032	**Semiconductor Nanophotonics: Materials, Models, Devices - GaN based Photonics I: Polaritzation Fields**
DS 9.1–9.4	Mon	16:00–17:15	H 2032	**Semiconductor Nanophotonics: Materials, Models, Devices - GaN based Photonics II**
DS 10.1–10.5	Mon	17:30–19:00	H 2032	**Semiconductor Nanophotonics: Materials, Models, Devices - Novel Concepts**
DS 11.1–11.8	Tue	9:30–11:30	H 2013	**Thin Film Characterisation: Structure Analyse and Composition (XRD, TEM, XPS, SIMS, RBS, ...)**
DS 12.1–12.7	Tue	11:45–13:30	H 2013	**Thin Film Characterisation: Structure Analyse and Composition (XRD, TEM, XPS, SIMS, RBS, ...)**
DS 13.1–13.4	Tue	9:30–11:30	H 2032	**Optical Layers: Basic Research and Applications**
DS 14.1–14.3	Tue	12:00–13:30	H 2032	**Optical Layers: Basic Research and Applications**
DS 15.1–15.5	Tue	14:30–16:30	H 2032	**Functional Oxides**
DS 16.1–16.8	Tue	17:00–19:45	H 2032	**Functional Oxides**
DS 17.1–17.65	Tue	9:30–13:30	Poster A	**Poster: Trends in Ion Beam Technology, Magnetism in Thin Films, Functional Oxides, High-k Dielectric Materials, Semiconductor Nanophotonics, Nanoengineered Thin Films, Layer Deposition Processes, Layer Growth, Layer Properties, Thin Film Characterisation, Metal and Amorphous Layers, Application of Thin Films**
DS 18.1–18.39	Tue	14:30–19:30	Poster A	**Poster: Towards Molecular Spintronics, Organic Thin Films, Optical Layers, Vibrational Spectroscopy, Tayloring organic interfaces**
DS 19.1–19.11	Wed	14:30–17:30	H 2013	**Organic Interfaces (SYSA 6)**
DS 20.1–20.6	Wed	17:45–19:30	H 2013	**Organic Polymer-Metal Interfaces (SYSA 7)**
DS 21.1–21.6	Wed	14:30–16:30	H 2032	**High-k Dielectric Materials - Synthesis, Properties, Applications**
DS 22.1–22.5	Wed	16:45–18:30	H 2032	**High-k Dielectric Materials - Synthesis, Properties, Applications**
DS 23.1–23.12	Wed	18:30–20:30	Poster C	**High-k Dielectric Materials - Synthesis, Properties, Applications** **The posters can also be presented at Poster A on Tuesday morning (DS poster session).**
DS 24.1–24.3	Thu	9:30–11:00	H 2013	**Trends in Ion Beam Technology: From the Fundamentals to the Application**
DS 25.1–25.7	Thu	11:15–13:00	H 2013	**Trends in Ion Beam Technology: From the Fundamentals to the Application**
DS 26.1–26.1	Thu	13:45–14:15	H 2013	**Birkholz**
DS 27.1–27.3	Thu	14:30–16:00	H 2013	**Trends in Ion Beam Technology: From the Fundamentals to the Application**
DS 28.1–28.6	Thu	16:15–17:45	H 2013	**Trends in Ion Beam Technology: From the Fundamentals to the Application**
DS 29.1–29.6	Thu	18:00–19:30	H 2013	**Nanoengineered Thin Films**
DS 30.1–30.6	Thu	9:30–11:00	H 2032	**Layer Properties: Electrical, Optical and Mechanical Properties**
DS 31.1–31.5	Thu	11:15–12:30	H 2032	**Application of Thin Films**
DS 32.1–32.5	Thu	13:15–14:30	H 2032	**Metal and Amorphous Layers**
DS 33.1–33.3	Thu	14:45–15:30	H 2032	**Surface Modification**
DS 34.1–34.4	Thu	15:45–16:45	H 2032	**Hard and Superhard Coatings**
DS 35.1–35.5	Thu	17:00–18:30	H 2032	**Nanostructured block copolymer films (SYSA 8)**
DS 36.1–36.5	Fri	10:15–12:00	H 2013	**Vibrational Spectroscopy of Nanolayers with Optical Probes**

DS 37.1–37.4	Fri	13:30–15:00	H 2013	**Vibrational Spectroscopy of Nanolayers with Optical Probes**
DS 38.1–38.3	Fri	15:15–16:45	H 2013	**Vibrational Spectroscopy of Nanolayers with Optical Probes**
DS 39.1–39.5	Fri	10:15–12:00	H 2032	**Magnetism in Thin Films: Interaction Phenomena and Heterostructures**
DS 40.1–40.6	Fri	12:15–14:15	H 2032	**Magnetism in Thin Films: Interaction Phenomena and Heterostructures**
DS 41.1–41.6	Fri	14:30–16:00	H 2032	**Layer Deposition Processes**
DS 42.1–42.4	Fri	16:15–17:15	H 2032	**Layer Growth: Evolution of Structure and Simulation**

Annual General Meeting of the Thin Films Division (DS)

Wednesday 18:45–19:15 Room H 2032

Annual General Meeting of the German Vacuum Society (DVG)

Wednesday 19:15–19:45 Room H 2032

DS 1: Towards Molecular Spintronics

Time: Monday 9:30–11:30 Location: H 2013

Invited Talk DS 1.1 Mon 9:30 H 2013

Organic Spintronics five years later — •Carlo Taliani — Institure for Nanostructured Materials CNR, Bologna, Italy

The discovery of spin injection in organic semiconductors (OS) dates back to 2002 when we published the paper [1]. That defined the beginning of a new branch of science in which OS are active media for the most advanced frontier in electronics in which information rather than by charges are transported and manipulated by the polarization of spins. The application of OS, as weak spin scatterers, in spintronics started from the intuition that colossal magnetoresistance ceramic materials like LSMO and OS could form a suitable interface for spin injection but, for the development of the principle, it was essential to have, both the ability and the expertise to grow organic as well as inorganic thin films in the same scientific environment as we have at ISMN. We generated the first planar spin valve made by LSMO /sexythiophene/ LSMO and observed a large magnetoresistance (MR) at room temperature depending inversely with the channel length with a peak of 30% MR for 80 nm gap. Several groups have confirmed the discovery giving rise to a solid interdisciplinary community of chemists and physicists at the frontier between magnetism and semiconductivity. In this presentation I will give an overview of the advancement in this field with a special emphasis to the potentiality of novel hybrid organic/inorganic interfaces.

[1]Room temperature spin polarized injection in organic semiconductors by V. Dediu, M. Murgia, F.C, Matacotta, C.Taliani, and S. Barbanera, Solid State Commun. !22, (2002) 181.

Invited Talk DS 1.2 Mon 10:00 H 2013

Organic spintronics: can theory play a role? — •Stefano Sanvito — School of Physics and CRANN, Trinity College Dublin, IRELAND

The ability of manipulating electron spins in organic molecular materials offers a new and extremely tantalizing agenda for both spin- and molecular-electronics. This is mainly due to the unquestionable advantage of weak spin-orbit and hyperfine interactions in organic molecules, which leads to the possibility of preserving spin-coherence over long times and distances. Moreover novel experiments with magnetic molecules demonstrate the profound influence of the molecular magnetic degrees of freedom on the transport. Theory can play an important role in this field, since first principles methods allow us to make quantitative predictions without adjustable parameters. In this talk I will overview recent theoretical progress in the field, in particular in the area of spin-phenomena at the single-molecule level.

First I will discuss the feasibility of organic spin-valves. These can exhibit a large bias-dependent magnetoresistance, that can be engineered by an appropriate choice of molecules and anchoring groups. Then, I will turn my attention to magnetic molecules. I will show results for Mn12 sandwiched between magnetic and non-magnetic electrodes and demonstrate the influence of the magnetic spin-state on the transport properties of the device. This is a formidable theoretical challenges since the simulation cells contain more than 1,000 atoms.

Invited Talk DS 1.3 Mon 10:30 H 2013

Spintronic and electro-mechanical effects in single-molecule transistors — •Maarten R. Wegewijs — Institut für Festkörper-Forschung - Theorie 3, Forschungszentrum Jülich, 52425 Jülich, Germany — Institut für Theoretische Physik A, RWTH Aachen, 52056 Aachen, Germany

The ability to electrically control the current through a single molecule in a three-terminal device geometry has opened up exciting perspectives for single-molecule spintronics. For instance, we predicted transport effects related to the coherent magnetization tunneling in single-molecule magnets which exhibit substantial magnetic anisotropy. In particular, non-trivial Kondo effects allow for a complete determination of the magnetic properties of such a device by transport measurements [1].

Another key feature of single-molecule transistors is the coupling of the electric current to quantized vibrations. In this talk, we will show how internal vibrations of a molecular transistor may be correlated with the total spin. We show how the total spin length may be determined using Franck-Condon transport effects i.e. without using a magnetic field. Finally, we show how electric control of the molecular spin is made possible by current-driven vibrations of the molecule.

[1] M. R. Wegewijs, C. Romeike, H. Schoeller and W. Hofstetter, New J. Phys. 9 344, (2007).

DS 1.4 Mon 11:00 H 2013

Electrical detection of spin coherence in thin organic layers — •Sebastian Schäfer[1], Somaie Saremi[1], Wolfgang Harneit[1], Kati Hübener[1], and Konstantinos Fostiropoulos[2] — [1]Freie Universität Berlin, Institut für Experimentalphysik, Arnimallee 14, 14195 Berlin, Germany — [2]Hahn-Meitner-Institut Berlin, Abteilung Heterogene Materialsysteme, Glienicker Str. 100, 14109 Berlin, Germany

An experimental demonstration of electrical detection of coherent spin motion of weakly coupled, localized electron spins in thin Fullerene C_{60}-Films at room temperature is presented. Pulsed electrically detected magnetic resonance experiments on vertical photocurrents through Al/C_{60}/ZnO samples showed that an electron spin Rabi oscillation of $\approx 10^4$ spins is detected by transient current changes. The nature of possible microscopic mechanisms responsible for this spin to charge conversion as well as its implications for the readout of endohedral Fullerene (N@C_{60}) spin qubits are discussed. Furthermore, current experiments on thin layers relavant for organic photovoltaic devices are presented.

DS 1.5 Mon 11:15 H 2013

Spin-polarised charge carrier transportin Ni/Alq_3/Co structures — Martin Roggenbuck, •Andreas Opitz, and Wolfgang Brütting — Institute of Physics, University of Augsburg, Germany

The spin state of electrons can be utilised to extend the probabilities of electronic circuits. Organic semiconductors are materiales with high spin diffusion lengths and long spin relaxation times and therefore interesting candidates for spintronics. Recently, spin polarised transport has been reported for diode structures comprising Alq_3 as organic semiconductor sandwiched between two ferromagnetic electrodes [1].

In this work cobalt and nickel are used as electrode materials, which have a high work function and should be hole injecting. At low temperatures a negative magneto-resistance effect of $\Delta R/R \approx 4\%$ is observed. However, the measured I-V curves show a higher current in comparison to standard light-emitting devices, like ITO/PEDOT:PSS/Alq_3/LiF/Al. An analysis by secondary ion mass spectrometry confirms that cobalt diffuses into the Alq_3 layer up to a thickness of 70 nm. Furthermore small clusters appear on the Alq_3 film after cobalt deposition, as proven by scanning force and scanning electron microscopy. Nevertheless, the current of the device is still much higher than expected with regard to the reduced film thickness and the lower hole mobility than the electron mobility in Alq_3 [2]. This is an indication for a different origin of the magneto-resistance effect other than transport through the organic semiconductor.

[1] Z. H. Xiong, et al., *Nature* **427** (2004) 821.
[2] W. Brütting, et al., *Org. Electron.* **2** (2001) 1.

DS 2: Towards Molecular Spintronics

Time: Monday 11:45–13:45 Location: H 2013

Invited Talk DS 2.1 Mon 11:45 H 2013

Tunable electron spin resonance spectroscopy of multi-center paramagnetic molecular complexes in strong magnetic fields — •Vladislav Kataev — IFW Dresden, D-01171 Dresden

Determination of the low-energy spectrum of spin states and magnetic anisotropy is an important prerequisite on the route of functionalization of magnetically active molecular complexes for molecular based spintronics. Owing to the increasing complexity of the metal ion

polynuclear complexes which combine in a single molecule a large number of interacting transition metal ions, the resulting spin states have a large multiplicity and a complex structure. High magnetic field electron spin resonance (ESR) spectroscopy enbales to selectively tune different spin states into the resonance with external microwave radiation and thus to determine the relative energies of the spin levels as well as the magnitude and sign of the magnetic anisotropy. As an example, we will discuss our recent ESR and magnetization measurements of several novel molecular complexes whose magnetic cores are built of interacting paramagnetic 3*d*-ions , such as, e.g., $[L_2Ni_4(N_3)(O_2CAda)_4](ClO_4)$ and $[(L^2)Ni_2(\mu\text{-pydz})(N_3)_2](BPh_4)_2$. Experimental data give evidence that the ground state and magnetic anisotropy depend sensitively on the details of the intramolecular bonding geometry and ligand coordination that can be tuned by means of synthetic chemistry. Different spin states can be realized: (i) a nonmagnetic state which can be turned into a magnetic one in strong magnetic fields; (ii) a strongly magnetic ground state with substantial negative magnetic anisotropy, i.e. functionalities constitutive for applications in molecular based spintronics.

Invited Talk DS 2.2 Mon 12:15 H 2013

Coordinated metal centers: Single-molecule magnets and highspin to lowspin switching — •Paul Müller — Institut für Physik der Kondensierten Materie, Universität Erlangen-Nürnberg

Coordinated metal ions are the essential active centers of many molecules. They are quantum dots with an energy spectrum which can be tuned by the coordinating ligands. Even simple complexes with Mn, Fe, Co, or Cu centers show spectacular physical properties. The structural and electronic properties were studied at the single-molecule level by scanning-tunneling microscopy and current-imaging tunneling spectroscopy (CITS). We applied these methods to several single-molecule magnets and a spin-crossover polymer incorporating supramolecular Fe^{II} complexes. As the electronic density of states near the Fermi level is dominated by the metal 3d orbitals, CITS spectroscopy can visualize single metal ions in single-molecule magnets, even if these ions are embedded into the sheath of the organic ligand. Therefore, the magnetic state of these ions is accessible to spectroscopy with atomic resolution. CITS measurements of the spin-crossover polymer revealed a high conductivity contrast between monomers in the highspin and in the lowspin state, respectively. Spontaneous switching between these two states was also recorded. This work was done in collaboration with M.S. Alam, V. Dremov, T. Glaser, J. Kortus, Y. Koval, J.-M. Lehn, U. Mitra, A. Postnikov, M. Ruben, R. Saalfrank, M. Stocker, S. Strömsdörfer, and A. Volkov.

Invited Talk DS 2.3 Mon 12:45 H 2013

Substrate-induced magnetic ordering and switching of iron porphyrin molecules — •H. Wende[1], M. Bernien[2], J. Luo[2], C. Weis[1], N. Ponpandian[2], J. Kurde[2], J. Miguel[2], M. Piantek[2], X. Xu[2], Ph. Eckhold[2], W. Kuch[2], K. Baberschke[2], P. Srivastava[1], P.M. Panchmatia[3], B. Sanyal[3], P.M. Oppeneer[3], and O. Eriksson[3] — [1]Universität Duisburg-Essen, Fachbereich Physik — [2]Freie Universität Berlin, Fachbereich Physik — [3]Department of Physics, Uppsala University, Sweden

Paramagnetic porphyrin molecules in contact with a metallic substrate are promising as building blocks in molecular nano-electronics. For this purpose the manipulation of the spin of the central 3*d* atom in this biologically significant molecule is essential. Here, we study the structural orientation and the magnetic coupling of *in-situ* sublimated Fe porphyrin molecules on ferromagnetic Ni and Co films which are epitaxially grown on Cu(100). These studies utilize NEXAFS at the C and N K-edges, and XMCD at the Fe, Co and Ni $L_{2,3}$-edges, which provide element-specific magnetic properties. In a combined experimental-computational study we demonstrate that due to an indirect, super-exchange interaction between Fe atoms in the molecules and atoms in the substrate (Co or Ni) the paramagnetic molecules can be made to order ferromagnetically. The Fe magnetic moment can be rotated along directions in-plane as well as out-of-plane by a magnetization reversal of the substrate, thereby opening up an avenue for spin-dependent molecular electronics. Supported by BMBF (05KS4KEB5) and DFG (SFB 658, Heisenberg-Programm).

DS 2.4 Mon 13:15 H 2013

Controlling the magnetization direction in molecules via oxidation state — Atodiresei Nicolae[1], Peter H. Dederichs[1], Yuriy Mokrousov[2], Lars Bergqvist[1], Gustav Bihlmayer[1], and •Stefan Blügel[1] — [1]Institut für Festkörperforschung, Forschungszentrum Jülich, 52425 Jülich, Germany — [2]Institute for Applied Physics, University of Hamburg, 20355 Hamburg, Germany

By means of *ab initio* calculations we predict that it is possible to manipulate the magnetization direction in organic magnetic molecules by changing their oxidation state. We demonstrate this novel effect on the $Eu_2(C_8H_8)_3$ molecule, in which the hybridisation of the outer π-rings states with the Eu $4f$-states causes a redistribution of the orbitals around the Fermi level leading to a strong ferromagnetism due to a hole-mediated exchange mechanism. As a key result, we predict an oscillatory behavior of the easy axis of the magnetization as a function of the oxidation state of the molecule - a new effect, which could lead to revolutionary technological applications. Support by the DFG-SPP 1243 is gratefully acknowledged.

DS 2.5 Mon 13:30 H 2013

A first-principles DFT study of magnetic properties of a series of complexes based on a hexaaza-dithiophenolate ligand — •Claudia Loose[1], Eliseo Ruiz[2], Berthold Kersting[3], and Jens Kortus[1] — [1]Institut für Theoretische Physik, TU Bergakademie Freiberg, Leipziger Str. 23, D-09599 Freiberg, Germany — [2]Departament de Quimica Inorgánica and Institut de Recerca de Quimica Teórica i Computacional, Universitat de Barcelona, Diagonal 647,08028 Barcelona, Spain — [3]Institut für Anorganische Chemie, Universität Leipzig, Johannisallee 29, D-04103 Leipzig, Germany

We studied a series of complexes based on a hexaaza-dithiophenolate ligand by first-principles DFT as implemented in the all-electron NRL-MOL code. The main focus of our work was on the effect of different bridges and different metal centers on the magnetic exchange coupling. In agreement with experimental results we predict correctly ferromagnetic or antiferromagnetic coupling depending on bridge or metal center. Only in the case of Ni^{2+}-ions we find ferromagnetic coupling. The use of other metal centers results in a strong antiferromagnetic coupling.

Interestingly, the ferromagnetic coupling in case of Ni^{2+} complexes can be tuned by changing the third bridging ligand. Depending on the bridge the magnetic coupling can be changed between strong antiferromagnetic to strong ferromagnetic coupling. This behavior can be understood within the framework of the Hay-Thibeault-Hoffmann model, which relates the energies of the magnetic orbitals to the magnetic exchange coupling.

DS 3: Organic Thin Films

Time: Monday 14:30–16:00 Location: H 2013

DS 3.1 Mon 14:30 H 2013

Grain-boundary evolution in a pentacene monolayer — •Jian Zhang, Jürgen P. Rabe, and Norbert Koch — Institut für Physik, Humboldt-Universität zu Berlin, Newtonstrasse 15, D-12489 Berlin

Significant charge carrier trapping defects were shown to exist at grain boundaries (GBs) in polycrystalline pentacene films, and these GBs are the principal bottleneck for charge transport in organic thin-film transistors (OTFTs) and they also affect the overall lifetime of OTFTs. In order to better comprehend the growth of organic polycrystalline films and controlling the number of grain boundaries in these films, the formation and evolution of GBs in pentacene films has to be understood. In this work, the evolution of GBs in the first pentacene layer on SiO2 substrates was studied. Using transverse shear microscopy, we directly observed GBs within single pentacene topographical islands. These intra-island GBs form at very early stages of pentacene film growth (in the present case at a coverage of 0.05 ML). Consequently, the existence of GBs within single pentacene islands (not visible in height images) will complicate "single-grain" transport measurements. During island growth the intra-island GB density increases linearly, suggesting a continued formation of new grain boundaries also before islands coalesce. Additionally, post-fabrication thermal annealing can reduce the GB density significantly in the pentacene layer in direct

contact with SiO2, which should lead to a considerable decrease of charge carrier trapping sites in OTFTs.

DS 3.2 Mon 14:45 H 2013

In-situ growth studies of the organic semiconductors perfluoro-pentacene, pentacene, and diindenoperylene — •Stefan Kowarik[1], Alexander Gerlach[1], Alexander Hinderhofer[1], Frank Schreiber[1], Tushar Desai[2], Sukwon Hong[2], Aram Amassian[2], and James R. Engstrom[2] — [1]Universität Tübingen, Germany — [2]Cornell University, Ithaca, USA

We present x-ray data from real-time and in-situ growth monitoring for the molecule perfluoro-pentacene (PFP, an n-type semiconductor) and compare it to real-time growth-data for the popular systems pentacene (PEN, p-type) and diindenoperylene (DIP, p-type). For organic molecular beam deposition (OMBD) of PFP we show that 3d-growth sets in after two monolayers , i.e. earlier than for PEN and DIP which exhibit favorable layer-by-layer growth up to four and eight monolayers, respectively. In comparison to PEN and DIP which can exhibit coexistence of crystal structures within the temperature range of 10 - 70 °C, we find the PFP film structure to be very similar to its bulk structure and not compromised by occurrence of phase coexistence. Extending the possibilities of OMBD through deposition at hyperthermal energies, we show for the example of DIP that supersonic deposition of molecules can increase the in-plane island size.

DS 3.3 Mon 15:00 H 2013

Mixing and phase-separation in co-deposited films of rod-like conjugated molecules — •Jörn-Oliver Vogel[1], Ricarda Opitz[1], Ingo Salzmann[1], Steffen Duhm[1], Bert Nickel[2], Jürgen Rabe[1], and Norbert Koch[1] — [1]Humboldt-Universität zu Berlin, Berlin, Deutschland — [2]Ludwig-Maximilians-Universität, München, Deutschland

Pairs of rod-like conjugated molecular materials [sexithiophene (6T), p-sexiphenyl (6P), dihexylsexithiophene (DH6T), quaterthiophene (4T), and pentacene] were co-deposited by organic molecular beam deposition on silicon oxide. We studied the properties of thin film samples by atomic force microscopy (AFM), X-ray diffraction (XRD), and infrared spectroscopy (IR). The co-deposition of pairs of molecules with similarly sized conjugated cores (e.g., 6T/6P) resulted in layered structures with mutual intercalation of the molecules. In contrast, co-deposition of molecules with differently sized conjugated cores led to two different morphologies: (i) Pairs of non-alkylated molecules (e.g., 4T/6P) formed fibrous amorphous films. (ii) Pairs of alkylated and non-alkylated molecules (e.g., DH6T/4T) exhibited phase separation with crystalline structures comparable to the ones of the pure materials. Our results suggest that a similar size of the conjugated cores of two co-deposited molecular materials is a key prerequisite for the formation of layered structures with mutual intercalation of the molecules. The particular type of the conjugated molecular moiety seems not to play an important role.

DS 3.4 Mon 15:15 H 2013

Growth and characterization of thin films prepared from $F_{64}Pc$, a new class of organic molecular semiconductors — •Christopher Keil[1], Olga Tsaryova[2], Sergiu M. Gorun[2], Dieter Wöhrle[3], Olaf R. Hild[4], and Derck Schlettwein[1] — [1]Institut für Angewandte Physik, Justus-Liebig-Universität Gießen, Heinrich-Buff-Ring 16, D-35394 Gießen, Germany — [2]Department of Chemistry and Environmental Science, New Jersey Institute of Technology, University Heights, Newark, New Jersey 07102-1982, USA — [3]Institut für Organische und Makromolekulare Chemie, Universität Bremen, Leobener Strasse NW 2, D- 28334 Bremen, Germany — [4]Fraunhofer IPMS, Maria-Reiche-Str. 2, D-01445 Dresden, Germany

Thin films of the zinc, copper or vanadium-oxo complexes of $F_{64}Pc$, a perfluoro(isopropyl)phthalocyanine were prepared by physical vapor deposition in vacuum. Electrical conduction and optical transmission measurements were performed during the deposition of films to analyze the formation of conducting pathways, the mechanism of film growth and intermolecular electronic coupling. Transmission spectra of the films to a large extent resembled those of solutions of the molecules speaking in favor of widely decoupled molecules. A low extent of intermolecular electronic coupling was also concluded from the small specific conductivity $10^{-11} - 10^{-9}$ S cm^{-1}. A further decreasing specific conductivity upon exposure to air confirmed the n-type characteristics expected from the strongly electron- withdrawing characteristics of the perfluoro- alkyl substituents. The potential to apply this new class of molecular semiconductor materials in devices is discussed.

DS 3.5 Mon 15:30 H 2013

Morphological and electrical characterisation of discotic liquid crystals thin films — •Annalisa Calò[1], Pablo Stoliar[1], Massimiliano Cavallini[1], Yves Henri Geerts[2], and Fabio Biscarini[1] — [1]CNR-ISMN, Via Gobetti 101 Bologna (BO) 40129 Italy — [2]ULB, Laboratoire de Chimie des Polimères, CP 206/1, Boulevard du Triomphe, Brussels 1050 Belgium

In this work we study the correlation between the morphology and the electrical transport on thin films of H2Pc(OC14,10)4. Here we present a comprehensive morphological characterisation by means of both cross-polarisers optical microscopy (O.M.) and atomic force microscopy (AFM) changing the temperature across the different phases, i.e. columnar rectangular, columnar hexagonal, and melted phase. These microscopic techniques also provide information about the films stability depending on the interactions with the surface. We developed an in-situ experimental setup to obtain the electrical characterisation contemporary with the morphological study in order to study how the electrical transport relates to the molecular aggregation.

DS 3.6 Mon 15:45 H 2013

Quantitative evaluation of the anisotropy of the optical constants of phthalocyanine thin films — •Michael Fronk, Dietrich R.T. Zahn, and Georgeta Salvan — Physics Department, Chemnitz University of technology, D-09107 Chemnitz

In this work copper phthalocyanine films prepared by organic molecular beam deposition on silicon substrates with thicknesses of about 60 nm are investigated by means of variable angle spectroscopic ellipsometry (VASE) and reflection anisotropy spectroscopy (RAS). The ellipsometry results indicate an uniaxial symmetry of the organic films with the uniform optical constants in the film plane different from those out of plane. RAS shows in addition the presence of an in-plane optical anisotropy in the order of 10^{-3} to 10^{-2} that is too small to be detected by ellipsometry. The RAS data is analysed using the layer model "air - film - substrate". Considering that the incident light is composed of two parts polarised linearly parallel to the main axes of the in-plane anisotropy we calculate the difference of the optical constants of the organic film along the two axes. This allows to estimate the degree of preferential orientation of the molecules within the film plane.

DS 4: Organic Thin Films

Time: Monday 16:15–17:30 Location: H 2013

DS 4.1 Mon 16:15 H 2013

PTCDA on an alkali-halogenide layer: adsorption or formation of a complex? — •Hatice Karacuban, Sascha Koch, Thorsten Wagner, and Rolf Möller — Universität Duisburg-Essen, Fachbereich Physik, Lotharstr. 1-21, 47057 Duisburg

The initial growth of 3,4,9,10 perylene tetracarboxylic dianhydride (PTCDA) on a thin layer of NaCl was studied by means of scanning tunnelling microscopy (STM) in ultra high vacuum. The alkali-halogenide layer with a average coverage of 1.5 monolayer was prepared by thermal evaporation while the Cu(111) substrate held was at 345K. The local height of NaCl varies between 0, 2 and 3 layers. This thin insulating layer on Cu(111) still allows to establish a tunnelling current without dipping the tip into the surface. PTCDA was adsorbed on this surface. At a mean coverage of 0.04 monolayer, it was possible to image individual molecules attached to $< 011 >$ steps of the NaCl which are presumably sodium terminated. The alignment of the molecules at these steps can be explained by the partial charges of the molecules interacting with the steps. On terrasses which are not covered by NaCl and at a coverage of 0.4 monolayers, three phases are dominant where the molecules align parallel in rods. The rod phases contradict a simple Coulomb interaction between the molecules. How-

ever, this adsorption geometry can be explained by a complex formed between PTCDA molecules and sodium atoms.

DS 4.2 Mon 16:30 H 2013

Charged Molecules on Insulators: Optical Spectroscopy of PTCDA Ions — •Thomas Dienel, Andreas Krause, Roman Forker, and Torsten Fritz — Institut für Angewandte Photophysik, Technische Universität Dresden, 01062 Dresden, Germany

It has been shown that the performance of organic-based devices can be improved considerably by doping [1]. However, on the molecular scale the mechanisms of doping are still not fully understood. Here, optical spectroscopy comes in handy as valuable tool for material characterization. By applying *in situ* optical spectroscopy to (sub-)monolayer thick organic films during the actual doping process, insight in the successive development of the charged states can be gained.

In our contribution we present differential reflectance spectroscopy (DRS) [2] on perylene-3,4,9,10-tetracarboxylic-dianhydride (PTCDA) layers doped by potassium. From the spectral development with increasing potassium concentration we conclude the occurrence of different charged states and give reasons for their assignment.

[1] K. Walzer et al., Chem. Rev. **107** (2007), 1233.
[2] H. Proehl et al., Phys. Rev. B **71** (2005), 165207.

DS 4.3 Mon 16:45 H 2013

Electronic properties of thin halogenated perylene bisimide films on Ag(111). — •Markus Scholz[1], Stefan Krause[1], Rüdiger Schmidt[2], Frank Würthner[2], Achim Schöll[1], Friedrich Reinert[1], and Eberhard Umbach[1,3] — [1]Universität Würzburg, Experimentelle Physik II, 97074 Würzburg — [2]Universität Würzburg, Institut für Organische Chemie, 97074 Würzburg — [3]Forschungszentrum Karlsruhe, 76021 Karlsruhe

A majority of organic semiconductors exhibit p-channel behavior. For complementary circuits both p-type and n-type semiconductors are necessary. Perylene tetracarboxylic acid bisimides (PBI) are not only considered to be among the best n-type organic semiconductors available, but also their structural properties, e.g. the twist angle of the perylene core as well optical and electronic properties can be tuned by proper substituents at the perylene core.

While previous investigations on bay-substituted perylene bisimides were performed in solution or addressed the electron mobility in thin films, we focused on the electronic structure of thin condensed films of PBI-H4, core chlorinated PBI-Cl4, and core fluorinated PBI-F2 on Ag(111) substrates with x-ray and UV photoelectron spectroscopy (XPS/UPS) and inverse photoemission spectroscopy (IPES). Particular respect was given to the influence of different bay-substituents, which allow to vary the twist angle of the perylene core and thus possibly the intermolecular π-overlap. Additionally, the attenuation behavior of the substrate peaks allows conclusions about the growth mode.

DS 4.4 Mon 17:00 H 2013

Direct spectroscopic evidence for the π–π–interaction between heteroaromatic molecules — •F. Holch[1], D. Hübner[1], R. Fink[2], A. Schöll[1], F. Reinert[1], and E. Umbach[1] — [1]Universität Würzburg, Experimentelle Physik II — [2]Universität Erlangen/ICMM, Physikalische Chemie II

High-resolution near-edge x-ray absorption fine structure (NEXAFS) spectroscopy is a very sensitive tool to analyse the electronic structure of condensed, liquid, and gaseous samples. Moreover, it provides local information due to the localized core hole excitation. We have utilized the potentials of this technique to probe the localisation of the π–interaction within aggregates of organic molecules.

An analysis of the intermolecular interaction requires a comparison of high–quality spectroscopic data of gaseous and condensed organic molecules. On the example of the heteroaromatic molecules 1,4,5,8-naphthalene-tetracarboxylic acid dianhydride (NTCDA) and 3,4,9,10-perylene-tetracarboxylic acid dianhydride (PTCDA) we present spectroscopic evidence which allows us to confine the intermolecular interaction to the π–system of the aromatic core. The NEXAFS spectra show a consistent shift of all resonances of the naphthalene ring system towards lower energy upon condensation, while such a shift can not be observed for the functional group. These experimental findings can be interpreted in terms of a π–π–interaction induced delocalisation of the naphthalene π–system leading to a lowering of the respective orbital energy.

This project is financed by the BMBF under contract 05KS4WWC/2

DS 4.5 Mon 17:15 H 2013

Organic field effect transistors based on n-conducting PTCDI derivatives — •Daniel Lehmann and Dietrich R.T. Zahn — Chemnitz University of Technology, Semiconductor Physics, D-09107 Chemnitz, Germany

Perylenetetracarboxylic diimide (PTCDI) is a π-conjugated planar perylene derivative. Being used as a red dye pigment in industry, PTCDI is highly available, and due to its n-conducting properties it is a subject of interest as an organic semiconductor for organic field effect transistors (OFETs). We present a comparative study on the electrical properties of top contact OFETs based on different PTCDI derivatives: DiMethyl-PTCDI, DiPhenyl-PTCDI, DiMethoxyethyl-PTCDI, as well as Di3Pentyl-PTCDI. The gate oxide for the devices is a 100 nm thick layer of SiO_2 on a highly doped Si(100) substrate. The thickness of the organic layer is in all cases 20 nm. The top contacts were made by depositing gold through a shadow mask. Channel length and width are $L = 17 \ldots 186$ μm and $W = 3$ mm, respectively. While the initial electron mobility measured *in situ* is between 10^{-4} cm^2/Vs and 10^{-8} cm^2/Vs depending on the molecule, an annealing of the sample at about 100°C leads to an increase in mobility typically up to one order of magnitude. This mobility is stable and not influenceable by further bias stress. Furthermore, we report on the influence of air exposure, which leads to a breakdown of the mobility by several orders of magnitude.

DS 5: Organic Thin Films

Time: Monday 17:45–19:15 Location: H 2013

DS 5.1 Mon 17:45 H 2013

Functionalization of (0001) 6H-SiC with organic silanes — •Sebastian Schoell, Marco Hoeb, Ian Sharp, Martin Stutzmann, Martin Eickhoff, and Martin S. Brandt — Walter Schottky Institut, Technische Universität München, 85748 Garching, Germany

Due to its extraordinary physical properties and chemical stability SiC is a promising material for biosensor applications. The affinity of SiC to form OH-terminated surfaces by wet chemical treatments is exploited to generate functional layers via silanization with organic molecules on SiC. In particular, wet chemically processed layers of ODTMS and APDEMS on n-type (0001) 6H-SiC were investigated. The structural and chemical properties of these layers were studied by contact angle measurements, atomic force microscopy (AFM), thermal desorption spectroscopy (TDS), and X-ray photoelectron spectroscopy (XPS). The organic layers are smooth and change their wettablity depending on the molecules used. Desorption temperatures in the range of 550°C indicate covalent bonding of the organic molecules to the SiC surface. Starting from monolayers with amine functional groups, the possibility of attaching complex molecules was demonstrated by immobilizing proteins on micropatterned organic layers followed by direct imaging via fluorescence microscopy.

DS 5.2 Mon 18:00 H 2013

Electronic properties of self-assembled organic monolayers on Ge surfaces — •Ian Sharp, Sebastian Schoell, Marco Hoeb, Martin S. Brandt, and Martin Stutzmann — Walter Schottky Institut, Technische Universität München, 85748 Garching, Germany

Ge surfaces and interfaces are commonly characterized by high densities of electrically active defect centers which severely limit the performance of Ge-based devices. Here, we investigate the electrical properties of metal-insulator-semiconductor (MIS) structures consisting of self-assembled alkyl monolayer-based insulating layers. Alkylation of the surface is achieved via thermal hydrogermylation of hydrogen terminated n-type (100) and (111) Ge with 1-octadecene, which is analogous to the well-known hydrosilylation reaction on Si. Chemical and structural characterization by thermal desorption spectroscopy (TDS), water contact angle measurements, and x-ray photoelectron

spectroscopy (XPS) is performed and reveals covalently bound and tightly packed organic monolayers. Current-voltage (IV) measurements show strong rectifying behavior, although relatively large reverse bias saturation currents were observed. Capacitance-voltage (CV) measurements on both highly and nominally n-doped samples reveal Fermi-level pinning of functionalized surfaces at 0.2 eV below the conduction band edge. However, no slow-state charge trapping is observed and saturation capacitance behaviors are indicative of high quality insulating layers.

DS 5.3 Mon 18:15 H 2013

Anisotropic optical function of diindenoperylene thin films determined by ellipsometry — •Ute Heinemeyer[1], Reinhard Scholz[2], Linus Gisslen[2], M. Isabel Alonso[3], J. Oriol Ossó[3], Miquel Garriga[3], Alexander Gerlach[1], and Frank Schreiber[1] — [1]Institut für Angewandte Physik, Auf der Morgenstelle 10, 72076 Tübingen — [2]Walter Schottky Institut, Technische Universität München, Am Coulombwall 3, 85748 Garching — [3]Institut de Ciència de Materials de Barcelona, CSIC Esfera UAB, 08193 Bellaterra, Spain

Diindenoperylene (DIP) has received increased attention due to its well defined ordering and promising electronic transport properties. Furthermore DIP exhibits a well-defined vibronic progression of the HOMO-LUMO transition providing direct access to the exciton-phonon coupling. We investigate the optical properties of DIP thin films on Si-substrates by variable angle spectroscopic ellipsometry and compare the results with the absorption spectrum of monomers in solution. Since the molecules in the thin film phase are stacked in a highly ordered way the DIP films ($\approx$ 40 nm) exhibit strongly anisotropic optical properties with uniaxial symmetry. Due to this anisotropy, it is necessary to perform a multisample analysis in order to obtain the optical function reliably. This data analysis is discussed for the energy range from 1.25 to 3 eV. A part of the vibronic progression resembles the vibronic subbands of dissolved monomers, but the quantitative interpretation of additional features requires an analysis with a model allowing for the interference between neutral molecular excitations and intermolecular charge transfer transitions.

DS 5.4 Mon 18:30 H 2013

Exciton-phonon coupling in rubrene thin films — •Milan Kytka[1,2], Linus Gisslen[3], Alexander Gerlach[1], Jaroslav Kováč[2], Reinhard Scholz[3], and Frank Schreiber[1] — [1]Institut für Angewandte Physik, Auf der Morgenstelle 10, 72076 Tübingen — [2]Faculty of Electrical Engineering and Information Technology, Slovak University of Technology in Bratislava — [3]Walter Schottky Institut, Technische Universität München

We investigate the absorption spectra of amorphous rubrene thin films (thickness $\sim$30 nm) and rubrene molecules in solution using spectroscopic ellipsometry and UV-VIS spectroscopy, respectively. We evaporated purified rubrene material under UHV conditions and measured the optical constants $n + ik$ in-situ. Both for the solution and the thin films, we find a well-defined vibronic progression of the S_0–S_1 transition of rubrene, because of the small orbital overlap of the π-electrons in the tetracene backbone with the four phenyl groups. We present a detailed data analysis for the progression of the vibronic transitions in the thin film and in the solution. Employing the model of displaced harmonic oscillator we obtain the characteristic parameters of the first absorption band. Using B3LYP/DZ (DFT) calculations we find good agreement with the experimental data. We find that the variation of the electronic and vibrational energy as well as the slightly higher electron-phonon coupling may be assigned not only to intermolecular interactions, but also to a different conformation of the molecule in the thin film phase.

DS 5.5 Mon 18:45 H 2013

Reduced intermolecular interaction in organic ultra-thin films of α-NPD: A multi-sample analysis using VUV ellipsometry — •Sukumar Rudra[1], Cameliu Himcinschi[1], Sindu John Louis[1], Marion Friedrich[1], Christoph Cobet[2], Norbert Esser[2], and Dietrich r.t. Zahn[1] — [1]Technische Universität Chemnitz, Chemnitz, Germany — [2]Institute for Analytical Sciences, Berlin, Germany

In situ ellipsometry using synchrotron radiation in the vacuum ultraviolet (VUV) range was employed to study the growth of α-NPD films starting from submonolayer coverage to bulk-like thicknesses. α-NPD was deposited on hydrogen passivated silicon and on ZnO (either Zn side or O side polished) substrates under ultra-high vacuum condition by organic molecular beam deposition. Ellipsometry was used to study the evolution of the dielectric function of the layers as a function of thickness on H-Si. It was found that the VUV absorption maxima of the ultra-thin film in the submonolayer thickness are spectrally blueshifted compared to its bulk counterparts. To confirm the role of the substrate in the blueshift, it was further studied on two different faces of ZnO substrates and the same behaviour was observed even though the shift was reduced compared to that on H-Si. Reduced intermolecular interaction seems to be the dominant reason behind the shift, whereas the substrate dependence is attributed to the changes in the local field due to the different polarizing media.

DS 5.6 Mon 19:00 H 2013

Improved understanding of polythiophene photo-oxidation mechanism and the role of PMMA layers as diffusion barriers — •Holger Hintz[1], Hans Joachim Egelhaaf[2], Ulf Dettinger[1], Umut Aygül[1], Heiko Peisert[1], and Thomas Chassé[1] — [1]University of Tübingen, Institute for Theoretical and Physical Chemistry, Auf der Morgenstelle 8, D-72076 Tübingen — [2]Christian-Doppler Labor für oberflächenoptische Methoden, Johannes-Kepler University & Konarka Austria GmbH, Altenbergerstaße 69, A-4040 Linz

Polythiophene (P3HT) plays an important role in organic electronic devices. The stability of this material is still unsatisfactory and the degradation mechanism has not yet been fully understood. Investigations of the photo-oxidation of thin P3HT layers were performed under ambient conditions and under varying partial pressures of oxygen and water using Xenon light. The degradation kinetics were investigated using UV/VIS spectroscopy. A linear decrease of absorbance was observed under all experimental conditions. In the presence of water, the oxidation rate increased significantly. The deposition of thin PMMA films on top of the P3HT layers clearly lowered the degradation rate under ambient conditions. In order to understand this stabilizing effect, oxygen diffusion coefficients through the PMMA top layer were determined by monitoring the quenching kinetics of the fluorescence of the P3HT layer. It was attempted to rationalize the experimental results by numerical simulations of the degradation kinetics.

DS 6: Semiconductor Nanophotonics: Materials, Models, Devices - High Speed Photonics

Time: Monday 9:30–11:00 Location: H 2032

Invited Talk DS 6.1 Mon 9:30 H 2032

High Speed Nano-Photonics — •Gadi Eisenstein — Electrical Engineering Dept. Technion Haifa, Israel

Active optoelectronic devices based on nano structure gain media have the potential to completely revolutionize broad band communication applications.

In particular, quantum dot optical amplifiers and mode locked lasers make use of the extremely broad gain bandwidth of quantum dot material and enable numerous possibilities not possible with previous, lower dimensionality gain media.

This talk will survey the basic concepts governing those broad band properties and will present an overview of the state of art and predicted future performance.

DS 6.2 Mon 10:15 H 2032

Small-signal cross-gain modulation of quantum dot semiconductor optical amplifiers — •Sven Liebich, Christian Meuer, Matthias Laemmlin, Jungho Kim, and Dieter Bimberg — Institut fuer Festkoerperphysik, Technische Universitaet Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

Wavelength conversion based on cross-gain modulation (XGM) of semiconductor optical amplifiers (SOA) is of largest importance for future all optical networks. Using the non-linear gain characteristics of quantum dot (QD) based SOAs this technique will be used for optical signal processing. QD SOAs have shown ultra-fast gain recovery which is superior to quantum well or bulk SOAs [1]. Furthermore in QD SOAs no crosstalk is expected for wavelengths having a difference larger than

the homogeneous broadening. To measure the small-signal XGM of QD SOAs a sinusoidally modulated optical pump which saturates the QD SOA is amplified. This results in a modulation of the gain of the amplifier and subsequently superimposes an inverted modulation on a second cw-probe signal. The XGM is measured in the frequency range 50 MHz to 40 GHz with a variation of the operating parameters like SOA current and wavelength detuning. The 3dB-bandwidth of the XGM for optimum operating parameters is observed to exceed 40 GHz. In conclusion, by increasing the drive current the SOA can be modified from low to high cross talk enabling efficient wavelength conversion at high bit rates.

[1] S. Dommers, V. V. Temnov, U. Woggon, J. Gomis, J. Martinez-Pastor, M. Laemmlin and D. Bimberg, APL 90 (2007)

DS 6.3 Mon 10:30 H 2032

1500 nm MOVPE-Grown InP-Based Quantum Dot (QD) Emitters — •Harald Künzel, Dieter Franke, Peter Harde, Jochen Kreissl, and Martin Möhrle — Fraunhofer Institut für Nachrichtentechnik HHI, Einsteinufer 37, D-10587 Berlin

A present R&D task is to transfer the QD technology to InP-based GaInAsP materials for applications in the 1550 nm regime and beyond. Real QDs as successfully presently only achieved by conventional MOVPE have become one of the key techniques recently for emitter applications. The Stranski-Krastanow growth mode allows for the realisation of high densities of quite homogeneous QDs which in combination with stacking of uncoupled QD layers is a prerequisite to form the gain region in photonic devices. Furthermore, during implementation of such structures as active layers in laser structures thermal stability of the QDs during growth of the upper claddings was found to be severe problem most probably due to movement of In towards the QDs resulting in a marked blue-shift of the emission. This shift was systematically investigated using thermal treatment to simulate cladding growth. The strong dependence of the blue-shift of the QD emission on growth temperature is attributed to defects being incorporated during QD deposition. A careful adjustment of deposition conditions for stable emission and high QD density forms the basis for the fabrication of lasers with characteristics which as a whole are among the best achieved so far. Recent advances in lasers and epitaxial regrowth for BH-type optical amplifiers will be presented.

DS 6.4 Mon 10:45 H 2032

Relaxation oscillations in quantum dot lasers — •Ermin Malic[1], Kathy Lüdge[1], Moritz Bormann[1], Philipp Hövel[1], Matthias Kuntz[2], Dieter Bimberg[2], Andreas Knorr[1], and Eckehard Schöll[1] — [1]Institut für Theoretische Physik, TU Berlin, Hardenbergstr. 36, 10623 Berlin, Germany — [2]Institut für Festkörperphysik, TU Berlin

We present a theoretical simulation of the turn-on dynamics of electrically pumped InAs/GaAs quantum dot lasers. Our approach combines laser rate equations with microscopically calculated Coulomb scattering rates describing Auger transitions between localized quantum dot and continuous wetting layer states. The scattering rates are determined within the Boltzmann equation and within the orthogonalized plane wave approach. We go beyond the Hartree-Fock approximation and consider the Coulomb interaction up to the second order in the screened Coulomb potential.

Our simulations show the generation of relaxation oscillations in both the photon and charge carrier density dynamics. They start after a delay time of approximately 1ns that is due to the charge carrier filling of initially empty quantum dot states. The complex interplay between strongly nonlinear Coulomb scattering rates and radiative processes gives rise to the relaxation oscillations and determines their frequency and damping rate. In agreement with experiments, we obtain a strong damping of relaxation oscillations. Our results indicate the crucial importance of the Coulomb scattering processes for the understanding of the turn-on dynamics of quantum dot lasers.

DS 7: Semiconductor Nanophotonics: Materials, Models, Devices - Surface Emitters

Time: Monday 11:15–13:00 Location: H 2032

Invited Talk DS 7.1 Mon 11:15 H 2032

Recent advances of VCSEL photonics — •Fumio Koyama — Tokyo Institute of Technology, Yokohama 226-8503, Japan

A vertical cavity surface emitting laser (VCSEL) was invented 30 years ago. A lot of unique features have been proven, such as low power consumption, wafer-level testing, small packaging capability and so on. The market of VCSELs has been growing up rapidly in recent years and they are now key devices in local area networks using multi-mode optical fibers. Also, long wavelength VCSELs are currently attracting much interest for use in single-mode fiber metropolitan area and wide area network applications. In addition, a VCSEL-based disruptive technology enables various consumer applications such as a laser mouse and laser printers.

In this talk, the recent advance of VCSEL photonics will be reviewed, which include the wavelength engineering and integration of single-mode VCSEL arrays. The athermal operation of micromachined VCSELs is demonstrated. Also, this presentation explores the potential and challenges for new functions of VCSELs, including high-speed nonlinear phase-shifters, slow light modulators/switches and so on.

DS 7.2 Mon 12:00 H 2032

12.5 Gbit/s 1250 nm VCSELs Based on Low-Temperature Grown Highly Strained InGaAs — •F. Hopfer[1], A. Mutig[1], G. Fiol[1], M. Kuntz[1], V.A. Shchukin[1], N. N. Ledentsov[1], C. Bornholdt[3], S. S. Mikhrin[2], I. L. Krestnikov[2], D. A. Livshits[2], A. R. Kovsh[2], and D. Bimberg[1] — [1]Institut fuer Festkoerperphysik, Technische Universitaet Berlin, PN 5-2, Hardenbergstr. 36, 10623 Berlin, Germany — [2]Innolume GmbH, Konrad-Adenauer-Allee 11, 44263 Dortmund, Germany — [3]Fraunhofer Institut für Nachrichtentechnik, Heinrich-Hertz-Institut Berlin, Einsteinufer 37, 10587 Berlin, Germany

As frequencies increase, power consumption, signal attenuation, electromagnetic interference and crosstalk are limiting the performance of electrical interconnects. Optical solutions are thus increasingly considered for intrachip clock distribution and short distance chip-to-chip communication. For intra-chip applications the absorption of Si forces the emitters to operate above 1200 nm. Here we realized 12.5 Gb/s GaAs based VCSELs emitting at 1250 nm.

Multimode devices demonstrate at 25 °C a maximum modulation bandwidth of 8.5 GHz, their peak differential efficiency is 0.4 W/A. At the respective bias point the optical output power in a 65.5 muem multi mode fiber is 3 mW. Open eyes for a 12.5 Gb/s non-return-to-zero 2^31-1 pseudo random bit sequence at 25° C are achieved with a signal to noise ratio of 5.6. For single mode devices with a SMSR > 40 dB, the maximum modulation bandwidth at 25 °C is 9 GHz with a multimode fiber coupled optical output power of 1.5 mW.

DS 7.3 Mon 12:15 H 2032

First VECSELs based on quantum dots — •Johannes Pohl[1], Tim David Germann[1], André Strittmatter[1], Udo W. Pohl[1], Dieter Bimberg[1], Jussi Rautiainen[2], Mircea Guina[2], and Oleg G. Okhotnikov[2] — [1]Institute of Solid State Physics, TU Berlin, Germany — [2]ORC, Tampere University of Technology, Finland

Optically Pumped Vertical External Cavity Surface Emitting Lasers (OP-VECSELs) provide excellent beam quality as well as high power continuous-wave (cw) operation and the possibilty of intra-cavity second harmonic generation. Quantum Dots (QDs) are an attractive alternative to quantum wells due to their broad and flat gain spectrum and high temperature stability. However, no QD-based VECSEL devices are reported so far possibly due to the low modal gain of QD ensembles. The first QD-VECSELs are grown by metalorganic vapor-phase epitaxy with alternative precursors. Two completely different QD growth techniques are used for the VECSELs aiming at high modal gain. Sub-Monolayer (SML) deposition of InAs/GaAs layers provides ensembles with very high QD areal densities yielding high modal gain at ground state transition energy. These QDs were used to demonstrate the first SML-QD VECSEL with an output power of 1.4 W cw at 1034 nm. Growth in the Stranski-Krastanow (SK) regime provides a QD ensemble with a broad gain spectrum expanding the operational temperature range of the VECSEL. High modal gain values are obtained by matching the cavity resonance to excited state transitions of the QDs. The VECSEL based on InGaAs SK-QDs operates at 1040

nm with an output power of 280 mW cw.

Invited Talk DS 7.4 Mon 12:30 H 2032
Recent Advances on Long Wavelength VCSELs (> 1300 nm) — •Markus C. Amann — Walter Schottky Institut, Technische Universität München, D-85748 Garching, Germany

Recently, InP-based long-wavelength vertical-cavity surface-emitting lasers (VCSELs) based on buried tunnel junctions (BTJ VCSEL) achieved excellent performance for the entire 1300-2300nm wavelength range. With this device concept, a low-resistive tunnel junction enables the replacement of the major part of the p-doped layers by n-doped ones yielding ultra-low electrical resistances and reduced optical losses as well as a self-adjusted transverse photon and carrier confinement. This concept also allows the application of hybrid Au-dielectric Bragg mirrors with high index contrast and reflectivity. BTJ-VCSEL show sub-mA threshold currents, 0.9V threshold voltage (at 1550 nm), operation voltages below 1.2V, 30-70 ohm series resistance, differential efficiencies >25%, up to 3mW single-mode optical output power, >110°C cw operation, stable polarization and single-mode operation with SMSR of the order 50 dB. Electro-thermal wavelength-tuning over 4nm and micromechanical tuning over more than 40nm both in the continuous tuning-mode and with SMSR >30dB can be accomplished. Besides the device design and technology, we will discuss recent achievements on high-speed VCSELs and BTJ-VCSEL arrays and demonstrate experiments on broadband communications and spectroscopic trace-gas sensing.

DS 8: Semiconductor Nanophotonics: Materials, Models, Devices - GaN based Photonics I: Polaritzation Fields

Time: Monday 14:00–15:45 Location: H 2032

Invited Talk DS 8.1 Mon 14:00 H 2032
High Efficiency Nonpolar InGaN/GaN based Blue Light Emitting Diodes and Laser Diodes — •Steven P. DenBaars, Mathew C. Schmidt, Robert Farrell, Daniel Fezzell, Stacia Keller, James S. Speck, and Shuji Nakamura — Electrical and Computer Engineering and Materials Departments,University of California, Santa Barbara, California 93106, USA.

We report on the recent advances in the performance of nonpolar InGaN/GaN based blue light-emitting diodes (LEDs) grown on nonpolar a-plane and m-plane GaN. Significant improvement in the outputpower has been achieved by optimizing the growth conditions of the active region. Growth of nonpolar III-nitride based materials have attracted great attention in the recent years because of *polarization-free* heterostructures and the potential of improving the performance of (Al, Ga, In) N-based optoelectronic devices. However the poor structural quality of the planar a-plane and m-plane GaN templates limits the performance of the LEDs grown on them. In this work, we have studied thecontinuous wave (cw) and pulsed current performance of nonpolar InGaN/GaN LEDs and laser diodes grown on reduced defect bulk GaN.

High power and high efficiency nonpolar m-plane nitride light emitting diodes (LEDs) have been fabricated on low extended defect bulk m-plane GaN substrates. The LEDs were grown by metal organic chemical vapor deposition (MOCVD) using conditions similar to that of c-plane device growth. The output power and external quantum efficiency (EQE) of the packaged 300 - 300 mm^2 was 23.7 mW and 38.9%, respectively, at 20 mA. The peak wavelength was 407 nm and < 1 nm redshift was observed with change in drive current from 1* 20 mA. The EQE shows a minimal drop off at higher currents.

Recently we have employed these nonpolar (m-plane) InGaN/GaN quantum structures into laser diodes without any Al-containing waveguide cladding layers. These devices utilize thick InGaN quantum wells to generate transverse optical mode confinement and can be grown and fabricated in a manner analogous to InGaN/GaN light emitting diodes. Pulsed and CW lasing operation was demonstrated,with threshold current densities of 3.7 kA/cm^2 and 4.3 kA/cm^2, respectively.

This work was supported by the Solid State Lighting and Display Center (SSLDC) at the University of California Santa Barbara.

Invited Talk DS 8.2 Mon 14:45 H 2032
Polarization induced effects in GaN-based devices — •Oliver Ambacher — Fraunhofer Institute for Applied Solid State Physics, Tullastr. 72, D-79108 Freiburg, Germany

The macroscopic non-linear pyroelectric polarization of wurtzite AlGaN, InGaN and AlInN ternary compounds dramatically affects the optical and electrical properties of multilayered Al(In)GaN/GaN hetero-, nanostructures and devices, due to the huge built-in electrostatic fields and bound interface charges caused by gradients in polarization at surfaces and heterointerfaces. In the presentation we review the theoretical and experimental results of the elastic and pyroelectric properties of binary and ternary group-III-nitrides with wurtzite crystal structure. We develop an improved method to calculate the piezoelectric and spontaneous polarization taking non-linearities due to alloying and/or high internal strain into account. Polarization induced interface charges and sheet carrier concentrations of 2DEGs are predicted for pseudomorphic InGaN/GaN, AlGaN/GaN and AlInN/GaN quantum well and heterostructures on the basis of the improved theory and compared with experimental results achieved by a combination of elastic recoil detection, high resolution X-ray diffraction, X-ray standing wave, photoluminescence, C-V profiling, and Hall effect measurements. Based on the improved model of polarization induced surface and interface charges a review of novel sensors based on AlGaN/GaN-heterostructures is provided, enabling a detailed understanding of the detection mechanisms and new functionalities of these interesting devices.

Invited Talk DS 8.3 Mon 15:15 H 2032
The optoelectronic chameleon - GaN-based light emitters from the UV to green — •Michael Kneissl — Institut für Festkörperphysik, Technische Universität Berlin, Hardenbergstr. 36, D-10123 Berlin, Germany

Group III-nitrides have evolved into one of the most versatile and important semiconductor materials for optoelectronic devices. GaN-based blue, green and white light emitting diodes have already entered many parts of everyday life and violet lasers are expected to be following soon. However, considering the extraordinary electronic properties and the wide spectral range that is accessible through nitride materials, it appears that it we have just touched the tip of the iceberg. We will discuss some of the new fields of research for InAlGaN materials and devices and review progress in the development of near and deep ultraviolet light emitting diodes, as well as growth and optical properties of InN and indium rich InGaN alloys for emitter in the blue-green spectral range and beyond.

DS 9: Semiconductor Nanophotonics: Materials, Models, Devices - GaN based Photonics II

Time: Monday 16:00–17:15 Location: H 2032

Invited Talk DS 9.1 Mon 16:00 H 2032
GaN-Photonics on Silicon — •Alois Krost — Institute of Experimantal Physics, Otto-von-Guericke University Magdeburg

In spite of large efforts there is still a lack of available homosubstrates for group-III nitrides. Currently, GaN-based devices are usually grown on transparent sapphire or Silicon carbide substrates. These are either insulating or very expensive and not available in large diameter. Silicon is the substrate of choice because of its cheapness, availability of large and high-quality substrates combined with good thermal conductivity and insulating or conductive electrical properties. In the last years fundamental problems such as the huge thermal mismatch leading to cracks have been overcome by several approaches such as (Al,Ga)N

buffer layers, low-temperature AlN interlayers, or growth on patterned substrates. Most of the recent work and published device results have been for GaN growth on (111) silicon substrates, with the first commercial chips, mainly HEMTs, now available by several companies with diameters up to 150 mm. Meanwhile, we have also obtained the first MOVPE-grown, crack-free, GaN-based LED on (100) silicon after the insertion of multiple AlN interlayers in the buffer structure paving the way towards integrated optoelectronics with GaN-on-Silicon technology. However, for optoelectronics the situation is more challenging than with electronic applications because Si is a non-transparent substrate and 94 % of the generated light is absorbed. Thus, GaN-on-Si LEDs cannot compete with those on transparent substrates unless substrate removal is performed. Our latest results on this topic will be reported.

DS 9.2 Mon 16:30 H 2032

Analysis of the growth mechanisms for InGaN alloys in MOVPE — •Martin Leyer, J. Stellmach, M. Pristovsek, and M. Kneissl — Technische Universität Berlin, Institut für Festkörperphysik, Sekr. EW 6-1, Hardenbergstr. 36, 10623 Berlin

The realisation of light emitting devices and lasers in the green spectral range requires high quality InGaN layers with an Indium content of 20% or more. However, the growth of such is very challanging due to layers shows phenomena like binodal decomposition and strain, resulting in a significant reduction of the efficiency in these devices. To understand the mechanism of InGaN growth, thick (∼200 nm) layers were grown on GaN/sapphire templates. The growth temperature was systematically changed from 700°C to 800°C in 10°C steps. In-situ spectroscopic ellipsometry allowed to determine growth rate and surface roughness. XRD $\omega - 2\Theta$ measurements yield two main peaks up to growth temperatures of 790° C. The indium incorporation varies between 0.19%/°C for the first and 0.39%/°C for the second InGaN layer. Reciprocal space mapping around the (1 0 . 5) reflex revealed two growth regimes, indicating two different growth mechanisms. For temperatures above 750°C we found two fully strained InGaN layers. Below 750°C only the first InGaN layer was fully strained. At temperatures below 750°C first a fully strained layer grows up to a critical layer thickness. Exceeding this critical thickness the growth mode changes from 2D to 3D. Above 750°C an interplay of indium segregation and strain is the dominating process, resulting in the growth of fully strained InGaN layers with different indium content.

DS 9.3 Mon 16:45 H 2032

MOVPE grown Indium Nitride Quantum Dots — •C. Meissner[1,2], S. Ploch[1], M. Pristovsek[1], and M. Kneissl[1] — [1]Institut für Festkörperphysik, Technische Universität Berlin, Hardenbergstr. 36, EW6-1, 10623 Berlin — [2]ISAS - Institute for Analytical Sciences, Albert-Einstein-Str. 9, 12489 Berlin

Very little attention has been devoted to the growth of indium nitride quantum dots (InN QDs) despite a number of interesting applications, e.g. in infrared emitters or solar cells. We studied the growth of InN QDs on GaN/sapphire templates in a horizontal metalorganic vapor phase epitaxy (MOPVE) reactor investigated by in-situ spectroscopic ellipsometry (SE). The temperature, V/III ratio and growth time were systematically varied during InN quantum dot growth. In-situ ellipsometry allows us to observe the growth processes even for submonolayer coverages. After growth the samples were investigated by standard characterization methods like atomic force microscopy, high resolution x-ray diffraction and photoluminescence.

Our studies showed that growth temperatures between 500°C and 550°C and V/III ratios above 5000 yield quantum dot like structures. Immediately after TMIn flow is switched off the ellipsometry-transients exhibit a clear dip, what can be attributed to desorption of excess Indium or a ripening process. At lower growth temperatures the QD density increases to 10^{11} cm^{-2} while the size decreases with mean height of a few nanometer and diameters as small as 16 nm. We will also discuss first experiments to overgrow the InN QDs with a GaN layer, which is a prerequisite step for the application of QDs in optical devices.

DS 9.4 Mon 17:00 H 2032

Recombination Kinetics of Localized Excitons in InGaN/GaN Quantum Dots — •Momme Winkelnkemper, Mattias Dworzak, Till Bartel, Axel Hoffmann, and Dieter Bimberg — Technische Universität Berlin, Institut für Festkörperphysik, Hardenbergstraße 36, D-10623 Berlin, Germany

The suitability of InGaN/GaN heterostructures for optoelectronic devices is sensitively affected by the built-in piezo- and pyroelectric fields, which affect the emission wavelengths as well as recombination dynamics via the quantum-confined Stark effect. In the present work, we study the photoluminescence (PL) decay of InGaN/GaN quantum dots (QDs) and its dependence on the built-in piezo- and pyroelectric fields. The decay of the ensemble photoluminescence (PL) is found to be strongly non-exponential, while all single-QD measurements yield exponential decays. We show that the non-exponential decay of the ensemble PL is well explained with a broad distribution of excitonic lifetimes within the QD ensemble. Using an inverse Laplace transformation, we derive an energy-dependent decay-time distribution function, which agrees well with the single-QD decay times. Within the framework of eight-band k.p theory, we calculate the dependence of the radiative excitonic lifetimes on structural parameters, such as QD height, lateral diameter, and chemical composition. The built-in piezo- and pyroelectric fields cause a sensitive dependence of the radiative lifetimes on the exact QD geometry and composition, resulting in a broad lifetime distribution even for moderate variations of the QD structure.

DS 10: Semiconductor Nanophotonics: Materials, Models, Devices - Novel Concepts

Time: Monday 17:30–19:00 Location: H 2032

Invited Talk DS 10.1 Mon 17:30 H 2032

Nanotechnology based single-mode lasers for telecommunication and sensing — Martin Kamp, Sven Höfling, and •Alfred Forchel — Technische Physik, Universität Würzburg, Am Hubland, 97074 Würzburg

High-performance single-mode lasers are key devices for optical communication, spectroscopy and sensing applications. For InP laser structures, the fabrication of single-mode devices using distributed feedback (DFB) gratings is a well established technology. However, the transfer of this technology to lasers with gain materials such as quantum dots, dilute nitrides or quantum cascade structures is not straightforward.

In this talk, we present several alternative approaches for the realization of single-mode lasers based on a single epitaxial step and subsequent nano-patterning. Several types of feedback gratings, e.g. lateral metal gratings, deeply etched sidewall gratings, top-surface gratings and distributed Bragg reflectors will be discussed. In all cases, the gratings can be defined without a second epitaxial step, leading to a greatly simplified fabrication process. Tunable single-mode lasers can be realized by the use of multiple segments with different gratings.

Another route towards single-mode devices is the use of photonic crystals, which can be used to tailor the mode structure of a semiconductor laser. Similar to the devices with gratings, tunability can be achieved by dividing the laser resonator in multiple segments. Photonic crystal based devices also allow the integration of additional functional elements, such as wavelength monitors.

DS 10.2 Mon 18:00 H 2032

20 W high brightness beam emission from 850 nm edge emitting lasers based on longitudinal photonic band crystal — •Thorsten Kettler[1], Kristijan Posilovic[1], Jörg Fricke[2], Armin Ginolas[2], Udo W. Pohl[1], Vitaly A. Shchukin[1], Nikolai N. Ledentsov[1], Dieter Bimberg[1], Jan Jönsson[3], Markus Weyers[3], and Götz Erbert[2] — [1]Institut für Festkörperphysik, Technische Universität Berlin — [2]Ferdinand-Braun-Institut für Höchstfrequenztechnik — [3]TESAG, Three-Five Epitaxial Services AG

Conventional edge emitting lasers suffer from large vertical beam divergence and are limited in maximal output power due to a narrow modal spot size of the optical mode leading to catastrophic optical mirror damage. For many applications, e.g. telecommunications, optical storage, display technology, as pump sources or for direct material processing higher brightness than available hitherto is desirable. Improving brightness at low cost is thus a key issue in research and development. We present here results from GaAs based 850 nm lasers

with a one dimensional photonic band crystal (PBC) acting as an ultra broad waveguide as well as a mode filter. The structure features 4 QW and 16 periods of the PBC. It exhibits high internal efficiency of 93 % and low losses of 3 cm^{-1}, measured for broad area devices. Vertical single mode operation is observed for various stripe widths with far field divergence below 8°. A 50 μm wide, 1.3 mm long stripe shows a high differential efficiency of 71 % with maximal output power of 19.5 W, leading to a brightness being one of the best values ever reported.

DS 10.3 Mon 18:15 H 2032

High-power wavelength stabilized 970-nm-range Tilted Cavity Laser — •G. Fiol[1], L.Ya. Karachinsky[1,2], I.I. Novikov[2], M. Kuntz[1], Yu.M. Shernyakov[2], N.Yu. Gordeev[2], M.V. Maximov[2], V.A. Shchukin[1,2], N.N. Ledentsov[1,2], and D. Bimberg[1] — [1]Institut für Festkörperphysik, Technische Universität Berlin, EW 5-2, Hardenbergstr. 36, D-10623 Berlin, Germany — [2]A.F.Ioffe Physico-Technical Institute, Politekhnicheskaya 26, 194021, St.Petersburg, Russia

Tilted Cavity Lasers (TCL) present an unexpensive all-epitaxial alternative to DFB- or DBR-lasers for wavelength stabilization avoiding lithographie. Broad-area (100 micrometer) devices, based on a GaAs/GaAlAs waveguide and GaInAs quantum wells emitting in the 970 nm spectral range, showed high temperature stability of the lasing wavelength (0.13 nm/K), low threshold current density (300 A/cm^2), a high power operation ($>$ 7 W in pulsed mode and $>$ 1.5 W in continuous wave mode), a high spectral stability at high output power, and a narrow vertical far field beam divergence (FWHM $\approx$ 20 degrees). 4 mm wide ridge lasers demonstrated spatial and spectral single mode continuous wave (cw) operation with a side mode suppression ratio (SMSR) up to 41.3 dB. Small signal modulation bandwidth of 3 GHz with a resonance peak of 6 dB at the relaxation oscillation frequency was measured for a 870 micrometer long device. TCL modulation efficiency is 0.36 $GHz/(mA)^{1/2}$. S-parameter measurements indicate that much higher frequencies may be expected in case of more advanced processing and/or shorter cavity lengths.

DS 10.4 Mon 18:30 H 2032

Small-Signal Cross-Gain Modulation Dynamics of Quantum-Dot Semiconductor Optical Amplifiers — •Jungho Kim[1], Matthias Laemmlin[1], Christian Meuer[1], Sven Liebich[1], Dieter Bimberg[1], and Gadi Eisenstein[1,2] — [1]Institut fuer Festkoerperphysik, Technische Universitaet Berlin, EW 5-2, Hardenbergstr. 36, 10623 Berlin, Germany — [2]Electrical Engineering Department, Technion, Haifa 32000, Israel

Quantum dot (QD) semiconductor optical amplifiers (SOAs) have been intensively investigated as pattern-effect-free, high-speed wavelength converters based on cross-gain modulation (XGM). Although pattern-effect-free wavelength conversion at 10 Gbit/s was experimentally achieved due to the ultrafast recovery time of spectral hole burning (<1ps) [1] in the gain saturation region, a comprehensive understanding of the gain saturation mechanisms is still required for further performance improvement. In this paper, we investigate the high-speed small-signal XGM response of QD SOAs. We numerically solve multiple coupled rate equations, which describe carrier dynamics and optical interaction among an ensemble of inhomogeneously broadened QDs. The calculated small-signal XGM with various injection currents is well matched with the experimental results and elucidates how the dynamics of QD gain saturation can be affected by the amount of stored carriers at QD excited states.

[1] S. Dommers, V. V. Temnov, U. Woggon, J. Gomis, J. Martinez-Pastor, M. Laemmlin, and D. Bimberg, Appl. Phys. Lett., vol. 90, 033508, 2007.

DS 10.5 Mon 18:45 H 2032

Single Photons for Quantum Information — •Oliver Benson — Institut für Physik , Humboldt-Universität zu Berlin, Hausvogteiplatz 5-7, 10117 Berlin, Germany

Single Photons have been widely discussed as ideal carriers of the fundamental units of quantum information processing (QIP), the quantum bits. In proposals and first experimental realizations the role of photons is two-fold: First, in linear optical quantum computing (LOQC) the photons themselves as used to implement single- and two-qubit gates. Second, in quantum interfaces photons are merely used to transfer quantum information from one place to another or among different physical QIP systems.

In this contribution we introduce experimental components that are required to implement photons for both purposes. We will describe the design of efficient single photon detectors based on superconducting NbN. Additionally, we report on the realization of an interferometric time-bin encoding setup for narrow band single photons.

DS 11: Thin Film Characterisation: Structure Analyse and Composition (XRD, TEM, XPS, SIMS, RBS, ...)

Time: Tuesday 9:30–11:30 Location: H 2013

DS 11.1 Tue 9:30 H 2013

New possibilities in high sensitivity Low Energy Ion Scattering (LEIS) for probing the outermost atomic layer — •Thomas Grehl[1], Ewald Niehuis[1], Rik ter Veen[2], and Hidde Brongersma[2] — [1]ION-TOF GmbH, Heisenbergstr. 15, 48149 Münster, Germany — [2]Calipso BV, Den Dolech 2, 5612 AZ Eindhoven, The Netherlands

With a recently developed high sensitivity Low Energy Ion Scattering (LEIS) instrument, a range of new applications arises for this extremely surface sensitive analytical technique. Known capabilities of LEIS are the selective characterisation and quantification of the atomic composition of the outermost atomic layer, i. e. precisely the atoms that control properties like catalytic performance, adhesion, wetting, corrosion, etc.

New possibilities such as surface imaging, sputter as well as non-destructive (static) profiling and even higher sensitivity for light elements have been added. The energy range of the primary ion source of up to 8 keV allows an improved mass resolution, thus enabling a better separation of the heaviest elements. In addition, a time-of-flight filter dramatically improves the detection limit for light elements. This filter suppresses the signal arising from sputtered ions, while scattered ions reach the detection system unhindered.

In this contribution, we show the utilization of these new capabilities to a range of samples and applications. Furthermore, we will show how LEIS can benefit from the combination with the complementary technique Time-of-Flight Secondary Ion Mass Spectrometry (TOF-SIMS), which adds ppb - ppm sensitivity, lateral resolution of 100 nm and chemical information.

DS 11.2 Tue 9:45 H 2013

Non-destructive probing of the chemical state of buried TiO_x nanolayers — •Beatrix Pollakowski[1], Burkhard Beckhoff[1], Stefan Braun[2], Peter Gawlitza[2], Falk Reinhardt[1], and Gerhard Ulm[1] — [1]Physikalisch-Technische Bundesanstalt, Abbestr. 2-12, 10587 Berlin — [2]Fraunhofer Institut Werkstoff- und Strahltechnik, Winterbergstr. 28, 01277 Dresden

Near edge x-ray absorption fine structure (NEXAFS) in combination with grazing incidence x-ray fluorescence (GIXRF) analysis provides a good approach for a depth-sensitive characterization of buried nanolayers with respect to both elemental composition and speciation. This idea offers the specific advantage of a high tunability of the information depth. The GIXRF regime implicates the occurrence of the x-ray standing waves (XSW) field above, at and below the surface affecting directly influence on the total fluorescence yield (TFY). The XSW field and the resulting mean information depth are dependent on incident angle and photon energy. The variation of the photon energy during a NEXAFS study requires to correct the incident angle to keep the mean information depth constant. The sample system consists of several 30 nm Ti nanolayers oxidized to different extents and being buried below 5 nm C. The results of angular corrected Ti $L_{3,2}$ NEXAFS spectra exhibit an electronic structure presumably comparable to that measured in total electron yield (TEY) and confirm the potential of this method. GIXRF-NEXAFS provides a complementary approach to different non-destructive techniques based on electron detection, which can reach their limits for deeply buried thin layers.

DS 11.3 Tue 10:00 H 2013

100% epi-Ge layers on engineered oxide heterostructures on Si — •Peter Rodenbach[1], Alessandro Giussani[1], Jose Ignacio Pascual[2], Dorin Geiger[3], Hannes Lichte[3], Peter Storck[4], and Thomas Schroeder[1] — [1]IHP Microelectronics, Im Technologiepark 25, 15236 Frankfurt Oder — [2]Institut für Experimentalphysik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin — [3]Technical University Dresden, Zellescher Weg 16, 01062 Dresden — [4]Siltronic AG, Hans-Seidel-Platz 4, 81737 München

Gallium-arsenide is a promising candidate for photo-voltaic systems due to its high efficiency factor, but has been reserved to space applications, owing this fact to the tremendous production costs. By providing an affordable Ge layer as a GaAs substrate, this technology might take a big step towards terrestrial use. Our group chose a 100% Ge on insulator technology approach, by epitaxially grown Ge epilayers on engineered oxide heterostructures on top of the Si(111) material system. In this case a cubic praseodymium-oxide buffer film is utilized. The MBE grown heterostructure has been examined by in-situ RHEED and ex-situ XRR, which both prove the smoothness of the closed (111)-oriented Germanium epi-layer. Furthermore the determination of the structural composition by GIXRD and XRD polefigures show the single-crystalline and twin-free A-B-A stacking nature of the Si(111)-Pr oxide-Epi-Ge(111) system. In addition the defect behaviour, especially stacking faults, is discussed based on the results obtained by TEM.

DS 11.4 Tue 10:15 H 2013

Lattice engineering of dielectric heterostructures on Si by isomorphic oxide - on - oxide epitaxy — •Andreas Wilke[1], Olaf Seifarth[1], Ioan Costina[1], Rakesh Sohal[1], Peter Zaumseil[1], Jose Ignacio Pascual[2], Peter Storck[3], and Thomas Schroeder[1] — [1]IHP Microelectronics, Im Technologiepark 25, 15236 Frankfurt Oder — [2]Institut für Experimentalphysik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin — [3]Siltronic AG, Hans-Seidel Platz 4, 81737 München

We are examining a new mixed oxide buffer system for the integration of functional semiconductors via heteroepitaxy on the Si (111) material platform, namely the flexible isomorphic oxide - on - oxide epitaxy approach of Y2O3 on cubic Pr2O3 with the ability to tune the buffer lattice constant. Our GI-XRD measurements prove the growth of high quality single crystalline Y2O3 on the cubic Pr2O3 (111) / Si (111) support system. Depth profiling X-ray diffraction shows that the growth mechanism of Y2O3 on cubic Pr2O3 is determined by the formation of a transition layer with variable lattice parameters, either due to strain or due to an interface reaction. In order to elucidate this question, in-situ XPS, UPS and RHEED measurements were applied.

DS 11.5 Tue 10:30 H 2013

ToF-SIMS Analysis of thin $Al_{1-x}Si_xO_y$ layers — •Pawel Michalowski[1], Gert Jaschke[2], Jens Steinhoff[2], and Steffen Teichert[2] — [1]Fraunhofer Center Nanoelektronische Technologien, Dresden — [2]Qimonda, Dresden

Recent interest in manufacturing new generation of memory devices based on high-k materials requires parallel development of proper analytic techniques. This work focuses on Secondary Ion Mass Spectroscopy (SIMS) measurements on atomic layer deposited $Al_{1-x}Si_xO_y$ composite materials in form of thin films in range of 5-20 nm. SIMS is a very sensitive method for contamination monitoring. Based on standards created with Rutherford Backscattering Spectrometry (RBS) SIMS proved to be useful for identification of the composition of unknown samples. Recent measurements are aimed to determine diffusion of silicon from substrate into a sample during the annealing process. This work can also provide useful information which can help to deeply understand what processes occurs in the material during the annealing under different temperature conditions. SIMS is a very promising technique for multi-purpose characterization of different materials and further optimization of measurement conditions and proper interpretation of results will be performed.

DS 11.6 Tue 10:45 H 2013

X-ray Photoelectron diffraction study of thin epitaxial MnO films — •Christian Langheinrich[1], Mathias Nagel[2], Angelika Chassé[1], and Thomas Chassé[2] — [1]Martin-Luther-Universität Halle-Wittenberg, FB Physik, FG Theoretische Physik, 06099 Halle — [2]Eberhard-Karls-Universität Tübingen, Institut für Physikalische und Theoretische Chemie, Auf der Morgenstelle 8, 72076 Tübingen

Transition metal oxides reveal interesting properties due to their high electronic correlation and magnetic phenomena. The MnO/Ag(001) system is an interesting model system due to the high lattice mismatch (9*%). By choosing the optimal preparation method either pseudomorphic or relaxed growth of ultrathin MnO on Ag(001) can be obtained. Recently, evidence for a tetragonal distortion of initial MnO layers epitaxially grown on Ag has been provided from both XPD and XAS experiments but further understanding seems necessary [1, 2].

Here, XPD has been applied to investigate MnO(001) and Ag(001) bulk, as well as ultrathin epitaxial MnO films on Ag(001). Calculations have been performed within a multiple scattering cluster model in order to obtain the lattice parameters. An r-factor analysis indicates that the MnO films exhibits a tetragonal distortion and relaxes step by step to bulk MnO with thicker films. In addition we are able to show the relaxation in dependence on the film thickness.

[1] M. Nagel, I. Biswas, P. Nagel, E. Pellegrin, S. Schuppler, H. Peisert, T. Chassé, Phys. Rev. B 75 (2007) 195426

[2] A. Chassé, Ch. Langheinrich, F. Müller, S. Hüfner, Surf. Sci. (accepted)

DS 11.7 Tue 11:00 H 2013

The interplay of PVD growth parameter and nanostructuring of C:V and C:Co nanocomposites — •Markus Berndt, Gintautas Abrasonis, Matthias Krause, Arndt Mücklich, Andreas Kolitsch, and Wolfhard Möller — Institute of Ion Beam Physics and Materials Research, Forschungszentrum Dresden-Rossendorf,D-01314 Dresden, Germany

The growth regimes of C:V and C:Co nanocomposite thin films (metal content of $\approx$ 15 and 30 at.%) grown by ion beam co-sputtering in the temperature range of RT-500°C are investigated. X-ray diffraction (XRD), transmission electron microscopy (TEM) and Raman spectroscopy at two excitation wavelengths (532 nm and 785 nm) have been used to characterize the microstructure of carbon and metal coexisting constituents of the nanocomposites. In order to reveal the influence of the transition metal on the encapsulating matrix, pure carbon films were deposited at the same temperatures.

C:Co and C:V nanocomposites exhibit a fine-grained structure at deposition temperatures below 300°C. At higher temperatures C:Co films tend to form nanocolumns, whereas the globular structure is preserved for C:V. X-ray patterns show low degree of crystallinity of the nanoparticles in C:Co and C:V composites.

Raman spectroscopy results show that the presence of metal significantly enhances the formation of aromatic clusters. This enhancement occurs independently on metal nanoparticle size, shape and phase.

DS 11.8 Tue 11:15 H 2013

Herstellung und Charakterisierung von Monolagen von Cobalt-Platin-Nanopartikeln — •Denis Greshnykh, Vesna Aleksandrovic, Igor Randjelovic, Andreas Frömsdorf, Andreas Kornowski, Christian Klinke und Horst Weller — Universität Hamburg, Institut für Physikalische Chemie, Grindelallee 117, 20146 Hamburg

Langmuir-Blodgett-Methode wurde verwendet um ausgedehnte geschlossene Monolagen von Cobalt-Platin-Nanopartikeln herzustellen.

Die Morphologie der erhaltenen Filme wurde mittels Elektronnemikroskopie (SEM) und Kleinwinkel-Röntgen-Streuung (GISAXS) untersucht.

Gleichstrommessungen bei unterschiedlichen Temperaturen zeigten einen thermisch aktivierten Ladungstransport. SEM, GISAXS und elektrische Messungen spiegeln die geringe Größenverteilung und den hohen Ordnungsgrad der Filme über mehrere Millimeter wider.

DS 12: Thin Film Characterisation: Structure Analyse and Composition (XRD, TEM, XPS, SIMS, RBS, ...)

Time: Tuesday 11:45–13:30 Location: H 2013

DS 12.1 Tue 11:45 H 2013

Experimental determination of the IMFP of electrons in organic molecular solids — •Tina Graber, Stefan Krause, Achim Schöll, and Friedrich Th. Reinert — Universität Würzburg, Experimentelle Physik II, Am Hubland, 97074 Würzburg

A precise knowledge of the inelastic mean free path (IMPF) of electrons in matter is of crucial interest in many respects. If electron spectroscopic techniques are applied in surface and interface science the attenuation length of the involved electrons has to be well-known in order to gain information on, e.g., adsorbate film thickness or growth modes. The IMFP certainly depends on the respective material and on the electron kinetic energy. Whereas some experimental information is available for inorganic compounds the data is very scarce for organic materials. Moreover, there is not yet a uniform theoretical description of the IMPF and the loss mechanisms of electrons in organic films, although some calculations have been performed [1]. In this work we present a systematic experimental study on the IMFP of electrons in condensed PTCDA films by means of photo electron spectroscopy (PES) and applying the overlayer method. Since the control of the adlayer growth mode it is mandatory for a precise determination, the attenuation length PTCDA/Ag(111) was chosen as a model system. The results indicate a significant deviation of the experimental IMPF values from the universal curve, which is generally utilized as a zeroth order approximation for the electron mean free path, particularly for low electron energies. [1] Tanuma, S.,Powell, C. J., Penn, D. R., Surf. Int. Anal. 21, 165, 1993

DS 12.2 Tue 12:00 H 2013

Zeitaufgelöste Studien zum Transport von Alkali-Ionen durch dünne Polymerfilme — •Thomas Kolling, Andreas Schlemmer und Karl-Michael Weitzel — Fachbereich Chemie, Philipps Universität Marburg

Dünne Filmschichten und Membrane spielen in Forschung und Technik eine grosse Rolle, z. B. in der Mikroelektronik, Medizintechnik aber auch allgemein in der Oberflächenbearbeitung und -veredelung. Ausgehend von Studien zum integralen Transport von Caesium-Ionen durch dünne PPX - (Poly-Para-Xylene) Membrane beschreiben wir hier erste zeitaufgelöste Studien zum Transport einzelner Ionen durch eine entsprechende Membran. Dazu wurden dünne PPX-Membrane variabler Dicke (100 nm bis 2 μm) durch Plasma-Dampfabscheidung (CVD) präpariert. So erzeugte Membrane wurden anschließend in einer Ultrahochvakuumkammer "freistehend" positioniert und mit gepulsten Ionenstrahlen verschiedener Alkali-Ionen, z.B. Cs^+ und K^+ beschossen. Durch die Membran hindurchtretende Teilchen wurden mit einem Mikrokanalplattendetektor zeitaufgelöst nachgewiesen und bezüglich ihrer kinetischen Energie analysiert. Gegenwärtig kann die Pulsdauer des Ionenstrahls vom μs-Bereich bis zu 100 ns variiert werden. Bei den kürzesten Pulsdauern finden wir deutliche Hinweise auf Energiedissipation im Zuge diffusiven Transports.

DS 12.3 Tue 12:15 H 2013

Surface sensitive analysis of YBCO thin films — •Tetyana Shapoval, Sebastian Engel, Elke Backen, Dagmar Meier, Marina Gründlich, Ulrike Wolff, Volker Neu, Bernhard Holzapfel, and Ludwig Schultz — IFW Dresden, Institute for Metallic Materials, P.O. Box 270116, D-01171 Dresden, Germany

Successful cleaning and polishing of a set of $YBa_2Cu_3O_{7-\delta}$ (YBCO) thin films prepared by Pulsed Laser Deposition (PLD) and Chemical Solution Deposition (CSD) have been performed. The roughness of the films was reduced to a value of less than 5 nm, which opens a way to apply local surface sensitive techniques even on formerly very rough samples (some hundred nm peak-to-valley) such as CSD YBCO films. As one application flux lines of YBCO films were imaged with the Omicron Cryogenic SFM in MFM mode.

The knowledge about geometry and distribution of artificial nanodefects in the interior of the film is crucial for further improvement of superconducting properties of these materials. The above mentioned polishing procedure has been further developed to prepare smooth low angle wedges of such samples. This offers the possibility to obtain depth dependent information with different surface sensitive scanning techniques. A high resolution electron backscattered diffraction image on the polished wedge of CSD YBCO sample reveals the homogeneous distribution of non superconducting $BaHfO_3$ nanoparticles in the whole volume of the film.

DS 12.4 Tue 12:30 H 2013

Depth Resolved Doppler Broadening Measurement of Layered Al-Sn-Samples — •Philip Pikart[1,2], Martin Stadlbauer[1,2], Klaus Schreckenbach[1,2], and Christoph Hugenschmidt[1,2] — [1]TU Munich, Department of Physics E21, James-Franck-Strasse, 85478 Garching — [2]TU Munich, ZWE FRM II, Lichtenbergstrasse 1, 85748 Garching

The accumulation of positrons in a 2-dimensional layer of tin embedded in aluminum is examined by Doppler Broadening Spectroscopy (DBS). For this purpose samples are grown out of high purity materials consisting of a step-shaped layer (0.1 to 200 nm) of tin on a substrate of aluminum and covered by an aluminum layer of constant thickness (200 nm). The positron implantation profile is varied by different positron acceleration energies of up to 15 keV. The pre-thermal implantation profile of the monoenergetic positron beam is examined since the effect of thermal positron diffusion is less significant at tin layers thicker than 50 nm. At thin layers (< 50 nm), the positrons greatly accumulate either at the aluminum-tin interface or in the tin layer due to its higher positron affinity compared to aluminum. Thus a very high sensitivity of the measurement for low densities of tin is observed. Consequently from the experimental results, a sensitivity threshold for the detection of a low amount of tin in an aluminum matrix with DBS is determined. The DB results are compared to theory by an approximation for pre-thermal implantation in layered materials.

DS 12.5 Tue 12:45 H 2013

Growth of ultrathin Ni-Al alloyed layers on Ni(111): evidence for NiAl formation over a critical thickness of Ni3Al — •Séverine Le Moal[1], Didier Schmaus[2], and Camille Cohen[2] — [1]Institut für Physikalische und Theoretische Chemie, Universität Bonn, Wegelerstr. 12, 53115 Bonn, Germany — [2]Institut des NanoSciences de Paris, 140 rue de Lourmel, 75015 Paris, France

Ni-Al alloys are of great technological interest because of their mechanical and thermal properties (high hardness, high melting point). They also are resistant to corrosion, this latter property being due to the formation at their surface of a passive film of aluminium oxide that acts as a diffusion barrier. Ultrathin epitaxial oxides are also used as convenient supports for model catalysts. We have studied in detail the alloying process of thin Al layers deposited on Ni(111), under ultrahigh vacuum conditions, as a function of the deposited Al amount, the deposition and annealing temperatures and the annealing time. The use of many complementary techniques, either in situ in the UHV chamber connected to a Van de Graaff accelerator (Rutherford Backscattering Spectrometry, Ion Channelling, Nuclear Resonance Profiling,Low Energy Electron Diffraction, Auger Electron Spectroscopy), or ex situ (X-Ray Diffraction, Atomic Force Microscopy) enabled us to have detailed information on the morphology, the composition and the crystallographic structure of both the surface and the bulk of the alloyed layer. A transition in the alloying process has been evidenced: the formation of Ni3Al (fcc-L12) for Al deposits thinner than 5 ML is followed by the formation of NiAl (cc-B2) over this critical thickness.

DS 12.6 Tue 13:00 H 2013

Texture analysis on $CrSi_2$: Combining statistical and microscopical information — •Herbert Schletter[1], Steffen Schulze[1], Michael Hietschold[1], Koen De Keyser[2], Christophe Detavernier[2], Gunter Beddies[1], and Meiken Falke[1] — [1]Institute of Physics, University of Technology, 09107 Chemnitz, Germany — [2]Department of Solid State Physics, Ghent University, Belgium 9000

Thin films of $CrSi_2$ on Si(001) were investigated with regard to their texture. Besides the various known epitaxial relations, another type of texture, the so-called axiotaxy, was found. The latter one is characterized by a texture axis with a fixed orientation relative to the substrate common to all crystallites, while there is a rotational degree of freedom around this axis. In contrast to the well-known fiber texture, in case of axiotaxy this texture axis is inclined with respect to the substrate

normal leading to a parallel arrangement of low-index planes across the interface. In case of $CrSi_2$, planes of {100}-type are parallel to Si{110} planes, generating an interface structure with one-dimensional periodicity. Due to the energetic advantage resulting thereof, this kind of texture is believed to be a common feature in thin films. In order to reveal the texture of the thin films, electron backscatter diffraction (EBSD) was used. Statistical information on the orientation distribution were obtained and visualized in pole figures. On the other hand, because the measurement is carried out in an SEM, it is possible to assign the orientation to every point on the sample. Thus, information about the correlation between orientation of a crystal and its size and shape are available.

DS 12.7 Tue 13:15 H 2013

Thermal Stability of Cs Fullerides — •Daniel Löffler, Patrick Weis, Sharali Malik, Artur Böttcher, and Manfred Kappes — Institut für Physikalische Chemie, Universität Karlsruhe, 76131 Karlsruhe, Germany

Thermal stability of solid Cs fullerides fabricated under ultra high vacuum conditions has been investigated by means of thermal desorption spectroscopy, ultraviolet photoelectron spectroscopy and secondary electron microscopy. The incorporation of Cs atoms proceeds by the formation of Cs_xC_{60} grains. The stability of Cs_xC_{60} depends on the doping degree x, $1 \leq x \leq 6$. Weakly doped phases, $Cs_{x<4}C_{60}$, decompose in three channels manifested by C_{60} sublimation peaks, α at 570 K, β at 660-720 K and γ at 820-900 K. Channel α reveals the sublimation of C_{60} molecules from sample regions not involved in the formation of fulleride grains. Sublimation channel β represents thermal desorption of C_{60} molecules terminating Cs_xC_{60} grains, x=1-3. The latter result from the phase segregation $nC_{60}{}^{m-} \longleftrightarrow C_{60} + mC_{60}{}^{n-}$, m=2,3, n=m+1 as activated during heating the sample [1]. The binding energy of C_{60} cages to the grain surface has been found to vary slightly with x in the range from 1.75 eV up to 1.95 eV. Saturated Cs_xC_{60}, $4 \leq x \leq 6$, phases decompose only via channel γ by sublimation of Cs_xC_{60} cages.

[1] G. Klupp et al., Phys. Rev. B, 74 (2006) 195402

DS 13: Optical Layers: Basic Research and Applications

Time: Tuesday 9:30–11:30 Location: H 2032

Invited Talk DS 13.1 Tue 9:30 H 2032

Film Production Technologies — •Hans K. Pulker — Thin Film Technology, Institute of Ion Physics and Applied Physics, University of Innsbruck, Austria

Films of elements, alloys, composites, and chemical compounds can be formed on solid substrates by various wet and dry chemical and physical deposition technologies. Depending on the applied technique, depositions are performed on air or in environmentally controlled atmosphere, under reduced gas pressure or in vacuum. In this paper mainly physical vapour deposition (PVD) processes are considered, because they are the preferred technologies for film deposition in optics. Chemical vapour deposition (CVD) and wet chemical processes are important in only few variants for this purpose. PVD processes are performed under vacuum and are based principally on purely physical effects. Intentionally forced chemical reactions by adding reactive gas to the coating chamber are used to deposit stoichiometric chemical compound films in the reactive deposition process. The chemical reactivity is generally positively influenced by the presence of a gas discharge plasma. In modern ion and plasma processes, input of energy into the growing film by collision and momentum transfer of kinetically enhanced ions, atoms and molecules causes densification and improves besides optical quality also structural and mechanical film properties and environmental stability. All the processes are used to deposit coatings in the thickness range between few nanometers up to some microns. Single films or multilayers can be deposited homogeneously or with graded composition.

Invited Talk DS 13.2 Tue 10:15 H 2032

Innovative stationary and in-line sputter technologies for precision optical coatings — •Peter Frach, Hagen Bartzsch, Joern-Steffen Liebig, Joern Weber, and Volker Kirchhoff — Fraunhofer-Institut fuer Elektronenstrahl- und Plasmatechnik,Winterbergstr. 28, 01277 Dresden, Germany

In this paper different new concepts for precision optical and antireflective coatings deposited by reactive Pulse Magnetron Sputtering (PMS) are introduced. In the first part features of stationary coating technology using various reactive gases and gas mixtures will be explained. The precise control of gas flow and process conditions during reactive sputtering of a silicon target in a mixture of oxygen and nitrogen gas allows to deposit layer systems with stepwise or gradient variation of the refractive index. Examples of AR-coatings, rugate and different filters based on SixOyNz coatings could proof the required optical performance as well as several application relevant properties like low internal stress, low roughness, high stability at temperature and humidity changes and at high density laser pulses. The complete coating can be done highly efficient at only one deposition station without interruption of the plasma. In the second part of the paper a new in-line coating system for precision optics with very strict requirements on accuracy, thickness uniformity and reproducibility will be presented that is based on two highly stabilized Pulse Magnetron Sputtering stations and a precision substrate transport system combined with an intermediate in-situ measurement.

Invited Talk DS 13.3 Tue 10:45 H 2032

Novel Process Concepts for Ion Beam Sputtering Deposition — •Kai Starke[1,2], Henrik Ehlers[1], Marc Lappschies[1], Nils Beermann[1], and Detlev Ristau[1] — [1]Laser Zentrum Hannover e.V., Hannover, Germany — [2]Cutting Edge Coatings GmbH

The application of charged noble gas beams with high ion current densities is of special scientific and economic importance for the production of highest quality thin film coatings. The ion beam sputtering process is known for the production of functional coatings of extreme optical performance concerning spectral characteristics, optical losses and damage resistance. During recent years, a tremendous increase in layer thickness precision has been achieved on the basis of broad-band optical monitoring techniques. Even complex thin film designs such as thin film polarizers, multi-band fluorescence filters and chirped mirrors can be manufactured without trial coating runs. Furthermore, an innovative process adaptation allows for the composition of material mixtures by co-deposition of two dielectric materials. This technique opens the field of novel optical materials with tailored properties and new thin film designs strategies like Rugate-filters. E.g. for TixSi1-xO2-mixture coatings, a distinctly increased damage threshold for ns-NIR pulses and a higher temperature resistance have been observed.

DS 13.4 Tue 11:15 H 2032

Reproduction of natural structural colours in thin film coatings — •Mathias Kolle[1], Heather Whitney[2], Ulrich Wiesner[3], and Ullrich Steiner[1] — [1]Cavendish Laboratories, Department of Physics, Cambridge University, UK — [2]Department of Plant Sciences, University of Cambridge, UK — [3]Materials Science Department, University of Cornell, Ithaca, USA

For many organisms in nature intense and distinctive colours play an important role in inter- and intra-species communication. Thus striking colours are well developed in nature and the most impressive natural colours actually arise from micrometre- to nanometre-sized structures, which often consist of intrinsically transparent materials.

Most of the underlying physical principles that create colour from mere transparent materials are well understood and the challenge lies in applying them to create artificial replicas of natural structural colours.

Nature shows that outstanding colours result in general from a balanced combination of various optical effects. Likewise we aim to create coatings based on nature-similar structures that optimally exploit different optical effects such as multilayer interference, diffraction from lateral structures as well as fluorescence.

Efficient, simple procedures and a variety of polymers and inorganic materials are used and will be subject of this presentation. Such coatings promise a wide range of applications only to mention unique labels in security applications to protect for instance credit cards, passports or banknotes from forgery.

DS 14: Optical Layers: Basic Research and Applications

Time: Tuesday 12:00–13:30 Location: H 2032

Invited Talk DS 14.1 Tue 12:00 H 2032

Demands on Coating Technologies in the Optical Component Industry — •Marcus Serwazi — CORNING GmbH; Abraham Lincoln Strasse 30; D-65189 Wiesbaden; Germany

Based on the famous and allways interesting improvements of the coating technologies during the last years and the upcoming question for the next challenges in development it might be useful to focus on the day by day business processes handled in the coating departments in the optical component manufacturing industry. The author will show some examples of state of the art coating products and describe and summarize the process chain and the related difficulties which needs to be adressed by upcoming development projects if the 'coater' should be supported by this projects for his future success in this market. Today very powerful and sophisticated coating technologies (e.g. several sputtering technologies) are available but the decision which is the right or best technology is sometimes not driven by the overall technical capabilities of this new technologies. Other factors like cost of operation, throughput and process reliability sometimes might lead to the outcome that the best decision for the next investment is not the 'newest' and most delicate technology which might be available in the market. The author light up some of this additional factors and also give his personal opinion in what he believes what drives allways the decision for the 'best' coating technology and the related investments in the optical component manufacturing industry in our days. He tries to summarize what kind of technology independent specifications can be derived from this knowledge for future systems and investigations.

Invited Talk DS 14.2 Tue 12:30 H 2032

Optische Prüfverfahren für die Qualitätssicherung in der Schicht- und Oberflächentechnik — •Uwe Beck — BAM, Fachgruppe VI.4 Oberflächentechnologien, Unter den Eichen 87, 12205 Berlin

Optische Prüfverfahren sind prädestiniert für den Einsatz in der Qualitätssicherung, weil sie zerstörungsfrei, berührungslos und schnell Informationen komplexer Schicht- und Materialsysteme liefern. Von besonderem Interesse sind dabei Schichtdicken, topographische Merkmale (Rauheit, Welligkeit) und optische Materialkenngrößen (Brechungsindex, Extinktionskoeffizient).

Während Bauteile vom Typ Makro sind, haben Schichten und deren spezifische Ausprägungen (Herstellung, Defekte) Dimensionen vom Typ Mikro oder Nano. Von besonderem Interesse ist die ortsaufgelöste Identifikation von Merkmalen im Vergleich zur globalen Umgebung (Homogenität) oder bezüglich einer Referenzprobe (Reproduzierbarkeit). Gleiches trifft auf Vorher-Nachher-Analysen (Beanspruchung, Degradation) zu. Daher sind "Fingerabdrücke" der Oberfläche sowie Imaging- und Replika-Techniken von besonderer Bedeutung.

Es werden typische Einsatzgebiete optischer Prüfverfahren z.B. der spektralen Ellipsometrie (SE), der Streifenlichtprojektion (FP), der Weißlichtinterferenzmikroskopie (WLIM), der Atomkraftmikroskopie (AFM) und von Röntgenverfahren (RFA, XRR) vorgestellt. Der kombinierte Methodeneinsatz erlaubt die Validierung von Schichtdicken, Topographie- und Materialkenngrößen, was an ausgewählte Beispielen diskutiert wird.

Invited Talk DS 14.3 Tue 13:00 H 2032

Mixed oxide coatings for advanced fs-laser applications — •Marco Jupe[1], Marc Lappschies[1], Kai Starke[1], Detlev Ristau[1], Andrius Melninkaitis[2], Valdas Sirutkaitis[2], Igor Cravetchi[3], and Wolfgang Rudolph[3] — [1]Laser Zentrum Hannover, Hannover, Deutschland — [2]Laser Research Center, Vilnius University, Vilnius, Lithuania — [3]Department of Physics and Astronomy, University of New Mexico, Albuquerque, NM 87131, USA

A modified IBS-process was used to create mixtures of oxide coating materials. The process allows to manufacture new designs, whereas the important optical and electronic properties of the material can be varied in a wide range. Especially for ultra short pulse applications, higher damage thresholds can be achieved. In this paper, LIDT measurements of mixed and pure single layers are presented. The coatings were investigated at different wavelengths and in a wide pulse duration range. The results of the measurements confirm the empirical law of the linear LIDT dependency on the absorption gap. Based on this empirical law, the RISED concept was developed. From the data of the single layer measurements, an optimization of RISED optical components in the fs-regime will lead to even higher damage thresholds. Particularly, for high reflecting mirrors the damage threshold could be doubled for different dielectric coating materials. Additionally, the paper presents a theoretical analysis of the stack LIDT on the basis of the single layer properties.

DS 15: Functional Oxides

Time: Tuesday 14:30–16:30 Location: H 2032

Invited Talk DS 15.1 Tue 14:30 H 2032

The truth about ferromagnetic ZnO — •Kay Potzger[1], Shengqiang Zhou[1], Georg Talut[1], Karsten Kuepper[1], Helfried Reuther[1], Arndt Mücklich[1], Jörg Grenzer[1], Manfred Helm[1], Jürgen Fassbender[1], Heidemarie Schmidt[1], Quingyu Xu[1], and Michael Lorenz[2] — [1]Forschungszentrum Dresden-Rossendorf, Bautzner Landstrasse 128, 01328 Dresden — [2]Universität Leipzig, Institut für Experimentelle Physik II, Linnéstraße 5, 04103 Leipzig

The combination of magnetic and semiconducting properties in oxides is currently one of most popular fields in materials research. Besides the expected gain of knowledge about basic physics, such materials have a large application potential in spin electronics. We present a summary of our results on transition metal doping of ZnO single crystals and thin films by means of ion implantation. We found that none of the samples investigated represents a diluted magnetic semiconductor as predicted by theory [1]. Nevertheless, transition metal ions can be dispersed within the ZnO matrix residing on different sites within the lattice depending on initial preparation conditions. The observed ferromagnetism mainly originates from secondary phase formation (metals or inverted spinels). We discuss the potential of those granular structures in spin-electronics. Moreover, we highlight the suppression of secondary phase formation by means of deliberately lowering the crystalline quality prior to the doping. In that case, purely defect induced ferromagnetic properties are observed. The effect of spin doping of such a defect induced ferromagnet is discussed.

[1] K. Sato and H. Katayama-Yoshida, Physica E 10, 251 (2001).

Invited Talk DS 15.2 Tue 15:00 H 2032

ZnO-based Hetero- and Quantum Well Structures for Light-Emitting Applications — •Fritz Henneberger and Sergey Sadofev — Humboldt-Universität zu Berlin, Institut für Physik, Newtonstr. 15, 12489 Berlin

Molecular-beam epitaxial growth far from thermal equilibrium allows us to overcome the standard solubility limit and to alloy ZnO with MgO or CdO in strict wurtzite phase up to mole fractions of several 10 %. In this way, a band-gap range from 2.1 to 4.4 eV can be covered. For epitaxy on ZnO substrates, we observe rocking curve widths of the ternaries as small as 19 arcsec and pseudomorphic growth over several 100 nm. A clear layer-by-layer growth mode controlled by RHEED oscillations enables us the fabrication atomically smooth heterointerfaces and well-defined quantum well structures exhibiting prominent band-gap related light emission in the whole composition range. Strong built-in polarization fields are screened off by moderate optical pumping. On appropriately designed structures, laser action from the UV down to green wavelengths and up to room temperature is achieved. All these findings make ZnO-based heterostructures promising candidates for opto-electronic applications in the short-wavelength range.

Invited Talk DS 15.3 Tue 15:30 H 2032

Large Area Deposition of Transparent Conductive Oxide Films — •Bernd Szyszka, Volker Sittinger, Andreas Pflug, Stephan Ulrich, and Felix Horstmann — Fraunhofer IST, Bien-

roder Weg 54e, 38108 Braunschweig

Transparent and conductive oxide films such as tin doped indium oxide (ITO), fluorine or atimony doped tin oxide and aluminum doped zinc oxide are key components for optoelectronic devcies such as thin film solar cells and flat panel displays.

This paper gives and outline on the material science of TCO films with special emphasize on ZnO:Al films. These films can be deposited at low temperature by reactive AC magnetron sputtering from metallic Zn:Al targets. They are a cost effective alternative for front electrodes of a-Si:H solar cells and also for ITO for flat panel displays. Films with resistivity of * < 270 **cm and low absorption (k@550 nm < 2 x 10-3) have been grown on 100 x 60 cm2 glass substrates. The optical properties of these films are characterized by ellipsometry and spectral photometry. Advanced models based on the Gerlach Grosse theory are implemented for the evaluation of free electron properties. Structural investigations are performed using XRD, SEM and HRTEM.

DS 15.4 Tue 16:00 H 2032

Effect of isothermal annealing on electrical and optical properties of Al-doped ZnO films — •Mykola Vinnichenko, Anatoly Rogozin, Natalia Shevchenko, Andreas Kolitsch, and Wolfhardt Möller — Institut für Ionenstrahlphysik und Materialforschung, Forchungszentrum Dresden-Rossendorf, P.F. 510119, 01314 Dresden, Germany

The aim of present work is to investigate mechanisms of Al incorporation and its effects on electrical and optical properties of ZnO films. Highly c-axis textured polycrystalline thin films of insulating ZnO were implanted by 110 keV Al^+ ions and then annealed at 520 °C. The films were characterized by Hall effect, four-point probe, spectroscopic ellipsometry and x-ray diffraction techniques. The films are nanocrystalline in as-implanted state. Their dielectric function shows broadened features near the band gap energy and increased, compared to unimplanted films, absorption in the near IR and visible spectral range. If the implantation dose is below 2x10^{16} cm^{-2}, the free electron density, Ne, increases after annealing and the film resistivity decreases monotonously during annealing. If the dose is above 2x10^{16} cm^{-2}, Ne decreases after annealing while film resistivity reaches minimum and then increases during the treatment. The annealing decreases optical absorption in the near IR and visible and improves film crystallinity. The behavior of the film electrical properties may be explained by the interplay between oxygen vacancies formation and Al donor activation.

DS 15.5 Tue 16:15 H 2032

Laser-assisted deposition and element analysis of nanocomposite oxide thin films — •Johannes Pedarnig[1,2], Johannes Heitz[1,2], Thomas Stehrer[1,2], Bernhard Praher[1,2], Richard Viskup[1,2], Khurram Siraj[2], Andreas Moser[2], Angela Vlad[2], Marius Bodea[2], Dieter Bäuerle[2], N. Hari Babu[3], and David Cardwell[3] — [1]Christian Doppler Laboratory for Laser-Assisted Diagnostics, — [2]Institute of Applied Physics, Johannes Kepler University Linz, A-4040 Linz, Austria — [3]Department of Engineering and IRC in Superconductivity, University of Cambridge,

Functional oxide thin films are epitaxially grown by pulsed-laser deposition (PLD) method. High-Tc superconducting (HTS) films of enhanced critical current density Jc are deposited by laser ablation of $YBa_2Cu_3O_7$ (Y-123) ceramics containing $Y_2Ba_4CuMO_x$ (M-2411, M = Ag, Nb, Ru, Zr) nano-particles. The Jc enhancement of nanocomposite films depends on the secondary phase content of the ceramic targets. Piezoelectric oxides such as novel $GaPO_4$ and ZnO doped with Lithium and Aluminum are grown as thin films and double-layers.

The monitoring of deposition processes and the element analysis of layers and ceramics are performed by laser-induced break down spectroscopy (LIBS). The LIBS signals recorded in situ are stable for more than 10000 laser pulses employed for target ablation. The relative element concentration in thin films and ceramics is the same demonstrating stoichiometric ablation and transfer of the multi-component oxide materials.

DS 16: Functional Oxides

Time: Tuesday 17:00–19:45 Location: H 2032

Invited Talk DS 16.1 Tue 17:00 H 2032

Zinc Oxide Nanostructures: Optical resonators and lasing — •Klaus Thonke[1], Anton Reiser[1], Martin Schirra[1], Martin Feneberg[1], Guenther M. Prinz[1], Tobias Röder[1], Rolf Sauer[1], Johannes Fallert[2], Felix Stelzl[2], Heinz Kalt[2], Stefan Gsell[3], Matthias Schreck[3], and Bernd Stritzker[3] — [1]Institut für Halbleiterphysik, Universität Ulm, D-89069 Ulm — [2]Institut für Angewandte Physik, Universität Karlsruhe (TH), D-76128 Karlsruhe — [3]Experimentalphysik IV, Universität Augsburg, D-86135 Augsburg

ZnO allows to grow a wide variety of nanostructures: Simple nanoclusters, -wool, ribbons, comb- and tree-like structures, tetrapods, pillars etc. All kinds of growth methods are used like metal-organic vapour phase epitaxy, molecular beam epitaxy, magnetron sputtering, pulsed laser deposition, vapour deposition with or without catalysts, electrodeposition, spray pyrolysis, or even simple wet chemistry methods. For application as sensors and optoelectronic devices nano-pillars are of special interest. Best structural quality and purity can be obtained with high temperature-processes around 900°C. We will show here examples of rather well-faceted hexagonal pillars grown on sapphire and silicon/iridium (fcc) substrates. Performing CL with high spatial resolution on as-grown single pillars we find UV light standing waves in pillars with appropriate diameters. These pillars show competing well-resolved spectral laser modes. Time-resolved measurements reveal the transition from spontaneous to stimulated emission and allow to study the electron-hole plasma driven lasing dynamics in more detail.

DS 16.2 Tue 17:30 H 2032

Switching and microstructural characterization of a Pt/TiO_2/Pt capacitor stack as nonvolatile ReRAM — •Herbert Schroeder, Jun Miao, and Doo Seok Jeong — IEM im Institut für Festkörperforschung und CNI, Forschungszentrum Jülich GmbH, D-52425 Jülich

Switchable resistors are discussed as nonvolatile resistive memory (NV-ReRAM) devices for future ultra-large scale-integrated memory chips in cross-bar architecture because of their simple geometry. A large variety of candidates is presently under discussion including paraelectric oxides. We have produced metal/insulator/metal (MIM) capacitor stacks with thin TiO_2 films between platinum electrodes and investigated the electrical and microstructural properties. As they are highly insulating they have to be electroformed to show the desired memory switching. In this contribution detailed experimental data on electrical and microstructural characterization are presented in order to demonstrate correlations and conclude on mechanisms controlling the forming and the switching. Besides ex-situ, sequential investigations also first results on in-situ experiments in electron microscopes are reported, i.e. the electrical current/voltage was applied during observation in a SEM and TEM. Main results are: a) Both memory switching modes, the symmetrical unipolar switching and the asymmetrical bipolar switching have been observed dependent on the forming sequence. b) Using very thin, electron transparent top electrodes (10-30 nm) and thin TiO_2 film (27nm) we could observe localized structural changes dependent on the forming sequence and the polarity of the forming.

DS 16.3 Tue 17:45 H 2032

Sputter deposited $LiCoO_2$ films as cathode material in thin-film batteries — •Tobias Stockhoff, Frank Berkemeier, and Guido Schmitz — Institut für Materialphysik, Westfälische Wilhelms-Universität Münster, 48149 Münster (Westf.), Germany

$LiCoO_2$ films of a thickness between 50 and 200 nm are deposited onto a Si-substrate by ion beam sputtering using Ar as sputter gas. The films are prepared under different deposition conditions by varying substrate temperature and the partial pressure of the oxygen, respectively. The chemical, structural, and electrical properties of the films are studied by means of TEM, XRD, and electrical measurements. Analytical TEM shows an oxygen deficiency in films sputtered under pure argon atmosphere and demonstrates the increase of the oxygen content if films are sputtered under an argon-oxygen ratio of 1:2. Due to the increased oxygen content, a significant increase of the specific dc-conductivity of the layers of about two orders of magnitude is observed

in the electrical measurements. While at lower substrate temperatures XRD measurements show a film structure similar to the LT-phase of $LiCoO_2$, at a substrate temperature of $600°C$ and an oxygen-argon ratio of 3:2 the HT-phase of $LiCoO_2$ is found, preferential orientated in <00l> direction. An electrochemical analysis of the films proves their potential for application in electrochemical cells.

Invited Talk DS 16.4 Tue 18:00 H 2032

Electrochromic coatings and windows — •Sabine Heusing — INM-Leibniz-Institut für Neue Materialien gGmbH, Campus D2 2, D-66123 Saarbrücken, Germany, e-mail: sabine.heusing@inm-gmbh.de

Electrochromic (EC) windows, also called "smart windows", change their optical properties (transmittance or reflection) in a reversible manner when a voltage is applied and a current flows through them. Large EC glazing are of considerable interest for architectural, automotive and aeroplane applications in order to control the solar radiation entrance to save energy costs for air conditioning in summer and for heating in winter (especially for buildings and automotives) and also to add comfort factors like privacy and to avoid glare and fading. EC windows have usually the configuration glass/ TCO/ EC-layer(1)/ electrolyte/ EC-layer(2) or ion-storage (IS) layer/ TCO/ glass, whereby TCO means transparent conductive oxide as e.g. tin doped indium oxide (ITO). As EC layer different metal oxides as cathodic electrochromic tungsten oxide and niobium oxide or anodic electrochromic nickel oxide can be used. These materials change their transmission reversibly by reduction (or oxidation) and insertion (extraction) of small ions (e.g. H+, Li+). The most studied EC material is the tungsten oxide due to its high coloration efficiency. The electrochromic materials and the electro-optical methods for characterisation of the EC-layers and the EC-windows will be presented. Furthermore the different techniques for the production of EC-layers and EC-windows will be shown and an overview of the large area EC glazing on the market or in prototype production and their typical features will be given.

Invited Talk DS 16.5 Tue 18:30 H 2032

Semiconducting metal oxides for gas sensors — •Tilman Sauerwald and Thorsten Wagner — Institut für Angewandte Physik, Justus Liebig Universität Giessen, Germany

Gas sensors based on semiconducting metal oxides like SnO_{2-x}, WO_{3-x} and Ga_2O_{3-x} are useful devices for the detection of hydrocarbons e.g. solvents. The sensor effect is based on a change in conductivity of the material caused by chemical reactions on the surface. In ambient air the surface of the metal oxide is covered by adsorbed, negatively charged oxygen. This leads to a depletion of electrons close to the surface (typically ∼10 nm). In granular films (commonly used) the conductivity is determined by the resulting surface barrier. For optimal sensing properties the structural size has to be comparable to the size of the depletion layer. Such structures can be obtained by a classical sol-gel process but they are not thermally stable. Methods utilizing selfassembly processes like endo- and exotemplating produce highly ordered nanostructures with enhanced stability. The reactivity of the metal oxide surface depends on different properties such as the acidity/basicity or the coverage with surface oxygen. Different surface acidity can be obtained by using different metal oxides and surface additives, this can be used for selective detection of solvents. The coverage with surface oxygen can be modulated by the modulation of the density of bulk donors by electrochemical polarisation of the sensor film

DS 16.6 Tue 19:00 H 2032

Structure and electronic properties of Scandate/Titante multilayers determined by high-resolution TEM/STEM and EELS — Martina Luysberg[1], •David Avila[1], Markus Boese[1], Tassilo Heeg[2], and Jürgen Schubert[2] — [1]Institut für Festkörperforschung und Ernst Ruska-Centrum, Foschungszentrum Jülich, 52425 Jülich — [2]Institut für Bio- und Nanosysteme, Foschungszentrum Jülich, 52425 Jülich

Because of their large dielectric constant rare earth scandates are promising candidates for the replacement of conventional gate oxides in MOSFET devices. In addition, they have a large potential to serve as substrate material for the epitaxial growth of perovskites, which are strained according to the lattice mismatch. The strain engineering of earth alkali titanate layers allows to tune their dielectric properties.

Here we report on structural and electronic properties of epitaxially grown $DyScO_3/SrTiO_3$ multilayers. Aberration corrected, high resolution TEM reveals prefect epitaxial layers, and allows for measurements of the strain. Aberration corrected STEM in connection with high resolution EELS gives information about the chemical and electronic properties. In particular, the near edge fine structure of the titanium $L_{2,3}$-edge shows a reduced crystal field splitting within the strained STO layers compared to cubic STO substrates. These results will be discussed in view of ferroelectric properties.

DS 16.7 Tue 19:15 H 2032

Optical characterization of individual, thermally reduced graphene oxide sheets — Inhwa Jung[1], •Matthias Vaupel[2], Richard Piner[1], and Rod Ruoff[3] — [1]Dept of Mechanical Engineering, 2145 Sheridan Road, Northwestern University, Evanston, IL 60208-3111, USA — [2]Nanofilm Technologie GmbH, 37081 Göttingen, Germany — [3]Dept of Mechanical Engineering, The University of Texas, 1 University Station, C2200, Austin, TX 78712-0292, USA

Graphite oxide is a layered material that can be exfoliated to form stable colloidal suspensions in water. At an appropriate concentration, evaporation of droplets of such a colloidal suspension on a surface yields individual graphene oxide sheets. This material is of interest as a filler for nano-composites as well as for use in new paper-like materials. A few layers or even one single layer of graphene oxide, including in its reduced form, where the O/C ratio is lower than in graphene oxide, are of potential interest in device applications. The optical dispersion functions of the refractive index and extinction coefficient of graphene oxide were measured by imaging spectroscopic ellipsometry on single and triple layers of graphene oxide. The results are compared with the results from confocal microscopy [1]. Dispersion parameters of a heap of graphene oxide sheets were also measured by conventional spectroscopic ellipso- metry and fit as effective medium. The effect of thermal treatment of graphene oxide, which renders the material conductive and reduces layer thickness, was explained. [1] Jung, I.; Pelton, M.; Piner. R.; Dikin. D.; Stankovich, S.; Watcharotone, S.; Hausner, M.; Ruoff, R. S. Nano Lett. 2007, NL0714177.

DS 16.8 Tue 19:30 H 2032

Density functional investigation of the dielectric constant for bilayer graphene under electric field — •Ruijuan Xiao, Manfred Taut, Ferenc Tasnadi, and Manuel Richter — IFW Dresden, Germany

Single and bilayer graphene have attracted much current interest not only because of their novel electronic structure but also for their potential application in future electronic devices. Several methods have been reported to open an energy gap in bilayer graphene, including application of gate-voltage, which may allow to switch off the electric conduction in bilayer graphene devices. In the present work, we evaluated the gap width and the dielectric constant of bilayer graphene in an external electric field (E_{ext}) using the full-potential local-orbital (FPLO) code. We obtain a dielectric constant reaching a minimal of 2.76 when the E_{ext}=0.3 V/Å, then increasing with the E_{ext}, reaching 2.84 when the E_{ext}=0.8V/Å. The calculated gap width increases with the E_{ext}, reaching a saturated value of 0.26eV when the E_{ext}=0.8V/Å. We also studied the effect of layer distance on the gap and dielectric constant of this system. The calculations indicate that the dielectric constant decreases linearly with the reduction of distance between the two graphene layers.

DS 17: Poster: Trends in Ion Beam Technology, Magnetism in Thin Films, Functional Oxides, High-k Dielectric Materials, Semiconductor Nanophotonics, Nanoengineered Thin Films, Layer Deposition Processes, Layer Growth, Layer Properties, Thin Film Characterisation, Metal and Amorphous Layers, Application of Thin Films

Time: Tuesday 9:30–13:30 Location: Poster A

DS 17.1 Tue 9:30 Poster A

Assembly of the Göttingen Proton Microbeam — •Jonas Hartwig, Holger Schebela, Gerhard Faubel, Michael Uhrmacher, and Hans Hofsäss — II. Physikalisches Institut, Georg August Universität, Friedrich Hundt Platz 1 37075 Göttingen

A microbeam system was installed in the göttingen accelerator lab. The used ion beam source is a 3 MeV Pelletron accelerator. The system consists of a russian quadruplett lens system, two adjustable slits and a target chamber with a X-ray detector and two silicon particle detectors. Between object slit and lens system two pependicular capacitors are installed to scan the beam over the target. The data acquisition is performed by a MARCO MicroDas unit and MPSYS 4 as acquisition software. These components where formerly used in Freiburg by Prof. R. Brenn. The distance between object slit and lens system is about 8m and the distance between the lenses and the target is 40cm. With this geometrical setup the object should be demagnified by factor 20 if all interferring fields will be eliminated. We aim for a beam size of 1 micrometer. The system will be used for analytical purposes (especially microPIXE) and protonbeam writing. First test results will be presented.

DS 17.2 Tue 9:30 Poster A

Relaxation effects in NiMnSb-Half-Heusler thin films — •A. Stahl[1], C. Kumpf[1], and E. Umbach[1,2] — [1]Universität Würzburg, Experimentelle Physik II, 97074 Würzburg — [2]Forschungszentrum Karlsruhe, 76021 Karlsruhe

The Half-Heusler alloy NiMnSb is an important material which will possibly enable the fabrication of spintronic devices due to it's unusual half-metallic properties. It can be grown in high crystalline quality on InGaAs/InP substrates, however, as for all heteroepitaxial systems mechanical stress is an important factor which influences crystalline quality, film growth, and magnetic properties.

We present several series of x-ray measurements on MBE-grown NiMnSb thin films on InP(111) and InP(001) substrates. Reciprocal space mapping and x-ray reflectivity were measured using the six-circle-diffractometer at BW2, HASYLAB, Hamburg. Structural properties like the critical thickness for pseudomorphic growth, relaxation, and interface roughnesses are discussed. Caused by different substrate orientations the systems show differences in relaxation. Furthermore the influence of exposure to air was investigated by capping some of the samples.

DS 17.3 Tue 9:30 Poster A

Electron Microscopic Examinations of Nickel Silicides — Meiken Falke[1], •Thomas Schaarschmidt[1], Maureen MacKenzie[2], Gunter Beddies[1], Steffen Schulze[1], and Michael Hietschold[1] — [1]TU Chemnitz, Deutschland — [2]University of Glasgow, UK

NiSi is a promising material for electrical contacts and interconnections in the latest generation of CMOS devices [1]. However there is a lack of information especially about chemical or structural variations in nanometer scale compounds. Due to the progressing miniaturisation knowledge of such variations is crucial for the successful adoption of these materials. Another important aspect is the thermal stability of the low-resistivity NiSi phase which generally changes into NiSi2 at a temperature of 700°C. This phase transformation can be shifted towards higher temperatures by alloying with Pt [2]. Ni films on a Si(001) substrate were sputtered together with Pt under different conditions to achieve various Pt concentrations and subsequently heated at selected temperatures. The resulting Ni-Pt-Si layers were investigated by electron microscopy. EDX and EELS measurements were applied to study the elemental composition within the layers. A recent work [3] has shown that it is possible to distinguish between different pure nickel silicide phases because of a shift of the Ni-L2,3 edge in EELS spectra. A similar edge shift could be observed for the different Ni-Pt-Si phases at hand.

[1] Lavoie, C., et al., Microelectronic Engineering, 2003 [2] Mangelinck, D., et al., Applied Physics Letters, 1999 [3] Cheynet, M.C., Pantel, R., Micron, 2006 Acknowledgement: DAAD D/07/09995

DS 17.4 Tue 9:30 Poster A

Investigation of the system C_{60}/ITO by X-ray absorption and resonant X-ray emission spectroscopy — •Karl Heinz Hallmeier[1], Daniel Wett[1], Reinhard Denecke[1], Iver Lauermann[2], Konstantinos Fostiropoulos[2], and Boyan Johnev[2] — [1]Wilhelm-Ostwald-Institut, Universität Leipzig, Linnéstr. 2, D-04103 Leipzig — [2]Hahn-Meitner-Institut Berlin GmbH, Dep. SE 2, Glienicker Str. 100, D-14109 Berlin

The system C_{60}/ITO is currently used to develop organic solar cells. In order to characterize this system, X-ray absorption spectroscopy in the total electron yield mode (TEY) and resonant X-ray emission spectroscopy (XES) in dependence of the polarization of the incoming beam have been performed at BESSY II (beamline U41-PGM) using the spectroscopic apparatus ROSA. In the present study we investigated layers of 50 nm C_{60} on ITO substrates, deposited by vacuum thermal evaporation of commercially available powders from graphite crucibles. While all our resonant (and non-resonant) XES data are identical to the spectra for free C_{60} powder [1] and also the first four absorption lines in the TEY spectrum agree, distinct differences appear in the high-energy (continuum) region. Possible explanations are electronic interactions resulting in a dipole between the uppermost ITO atoms (preferentially oxygen) and carbon atoms from a C_{60} molecule, or structural effects resulting from (multiple) backscattering of electrons excited from the carbon 1s level by the uppermost atoms of the ITO substrate. Financial support by DFG (FG 404-SZ58/15).
[1] J. Guo, J. Nordgren, J. Electr. Spectr. Rel. Phen., 110 (2000) 105.

DS 17.5 Tue 9:30 Poster A

Zur Bildung von Ni-Hydriden in reaktiven Plasmen — •Marion Quaas[1], Harm Wulff[1], Oxana Ivanova[2] und Christiane A. Helm[2] — [1]Institut für Biochemie, Universität Greifswald, Felix-Hausdorff-Straße 4, 17487 Greifswald — [2]Institut für Physik, Universität Greifswald, Felix-Hausdorff-Staße 6, 17487 Greifswald

20 nm dicke Ni-Filme mit einer mittleren Domänengröße von 7 nm werden in einem Mikrowellen-Plasma (SLAN, 700W) in einem Gasgemisch von 10 sccm Ar/ 10 sccm H_2 mit verschiedenen negativen Substratvorspannungen behandelt. Die Bildung fester kristalliner Ni-Hydride und die kinetischen Prozesse bei der Plasma-Wand-Wechselwirkung werden durch die Kombination von Röntgendiffraktometrie im streifenden Einfall (GIXD), Röntgenreflektometrie (XR) und Atomkraftmikroskopie (AFM) untersucht.

In Abhängigkeit vom Ionenenergieeinstrom entstehen verschiedene Reaktionsprodukte. Ohne Substratvorspannung entsteht kein Ni-Hydrid. Lediglich partielles Verdampfen/Sputtern und ein Kristallwachstum kleiner Ni-Domänen werden beobachtet. Bis -25 V bildet sich Ni_2H, bei -50 V wandelt sich das Ni_2H zu NiH um, bei -75 V entsteht direkt NiH.

Die Ni_2H-Bildung erfolgt schnell, der Wachstumsprozeß der NiH-Phase wird durch die Vorspannung beeinflusst.

Die kinetischen Prozesse werden quantifiziert und diskutiert.

DS 17.6 Tue 9:30 Poster A

Quantification of Impurities in ZnO — Niklas Volbers[1], •Andreas Laufer[1], Bruno K. Meyer[1], and Kay Potzger[2] — [1]1. Physics Institute, Justus-Liebig University Giessen, Heinrich-Buff-Ring 16, D-35392 Giessen, Germany — [2]Institute for Ion Beam Physics and Materials Research, Forschungszentrum Dresden-Rossendorf, PO Box 51 01 19, D-01314 Dresden, Germany

Current research on zinc oxide (ZnO) focuses on bipolar doping. The severe difficulties in obtaining p-type ZnO have been partially attributed to intrinsic defects and impurities that act as compensating donors. To avoid these effects, it is therefore necessary to identify the impurities in the material. Among the methods for impurity analysis, secondary ion mass spectrometry (SIMS) is very attractive due to the fact that the chemical identity of the elements can be determined directly, independent of factors such as the ionisation state or binding type. In addition, the sensitivities are very high enabling one to detect some elements in concentrations of as little as a few ppm. The quantification of SIMS data is possible using the method of relative sensitivity factors (RSF). Unfortunately, these factors vary for each host crystal and while there are RSF tables for Si and for compound semiconductors such as GaAs, InP or GaN, such a reference did not yet exist for ZnO. In the presented work, the RSF for a number of technological important elements have been determined, thus allowing one to quantify the impurity concentrations found. These factors have then been applied to ZnO crystals and thin films.

DS 17.7 Tue 9:30 Poster A

X-ray absorption spectroscopy of Prussian Blue analogues thin films — •Sébastien Bonhommeau, Niko Pontius, Hermann A. Dürr, and Wolfgang Eberhardt — Berliner Elektronenspeicherring-Gesellshaft für Synchrotronstrahlung m.b.H (BESSY), Albert-Einstein-Straße 15, 12489 Berlin, Germany

Prussian Blue (PB) was described for the first time in 1704. Since then, spectacular electrochemical, magnetic and photomagnetic prop-

erties have been revealed in PB and its analogues. In particular, CoFe PB analogues may display unusual photomagnetic effects arising from a light-induced Co(III)(low spin, S=0)-CN-Fe(II)(low spin, S=0) → Co(II)(high spin, S=3/2)-CN-Fe(III)(low spin, S=1/2) electron transfer accompanied by a spin change of Co. On the other hand, MnFe PB analogues exhibit transitions between the cubic Fe(III)(low spin, S=1/2)-CN-Mn(II)(high spin, S=5/2) phase and the tetragonal Fe(II)(low spin, S=0)-CN-Mn(III)(high spin, S=2) phase due to a charge-transfer-induced Jahn-Teller distortion.

We present X-ray absorption measurements performed at BESSY on RbCoFe, NaCoFe and RbMnFe PB 200 nm-thin films deposited on top of silicon nitride membranes. The experimental spectra are analysed using simulations based on the multiplet theory to estimate the properties of these films (crystal field, charge transfer, etc) compared to powder samples as well as the number of photoexcited CoFe and MnFe pairs.

DS 17.8 Tue 9:30 Poster A

The QQDS magnetic spectrometer "Little John" for High Resolution Depth Profiling — •Marcel Kosmata, Rainer Grötzschel, Daniel Hanf, Chavkat Akhmadaliev, Axel Weise, and Maik Vieluf — Forschungszentrum Dresden-Rossendorf e. V.

The aim of the modified magnetic spectrometer *Little John* [Gil89] is to measure concentration profiles of light elements in thin layers with sub-nanometer depth resolution by Elastic Recoil Detection Analysis (ERDA). For these measurements heavy ions from the Rossendorf 5MV-Tandem accelerator are directed to the sample. The ejected recoil atoms are detected and energy analysed under forward angles. The depth resolution depends directly on the energy resolution of the spectrometer. High energy resolution can only be obtained using magnetic particle spectrometers, where the energy measurement is transformed in a position measurement at the focal plane. The depth scale is provided by the stopping power of energetic heavy ions moving in matter, the available data of which assume a dynamic charge state equilibrium due to electron loss and capture along the ion trajectory. In the case of ultrathin layers the path length of the particles are too short to achieve this equilibrium. Since magnetic spectrometers separate particles with identical energy but different charge states it is necessary to consider charge state dependent stopping cross sections for quantitative data analysis. Here only very few data are available in the literature. In this work we introduce an experimental setup at *Little John* for charge state distribution measurements of light heavy ions and present first results.

DS 17.9 Tue 9:30 Poster A

Characterization and elemental analysis of nano- and micro-dimensional structures using PIXE and RBS — •Christoph Meinecke, Matthias Brandt, Marius Grundmann, Jürgen Vogt, and Tilman Butz — Institute of Experimental Physics II, University Leipzig, Linnestr. 5, 04103 Leipzig

Due to the current research in materials science, like in semiconductor physics, the production of micro- and nanostructures raises more interest for basic researchers. The aim is to control the electronic, magnetic and optical properties by variation of the elemental composition and feature size. During the last few years we developed an elemental characterization of different micro- and nanostructures using ion beam analysis with an expected spatial resolution of 100 nm, which is unique in the world.

New analytical experiments using focused high energy ion beams can reveal, apart from to stoichiometry and morphology, also the lattice structure of the micro- and nanostructures. The application of ion channeling like channeling-RBS and channeling-STIM to these new nanostructures, reveals lattice distortions.

This project characterizes sub-micrometer structures of different shapes and compositions (heterostructures, coated structures, homogeneous doped structures etc.) to learn more about growth procedures, electronic and magnetic properties, elemental distributions of multilayered microstructures and crystal quality using focused high energy ions.

DS 17.10 Tue 9:30 Poster A

Spray Pyrolysis as a deposition method for metal-oxide-particles — •Alexandre Santos Abreu[1], Christian Berthold[1], Matthias Knoll[1,2], Armin Konrad[2], Reinhard Tidecks[1], and Siegfried Horn[1] — [1]Universität Augsburg, Institut für Physik, EP II, Universitätsstr. 1, D-86159 Augsburg — [2]OSRAM GmbH, FL/CFL D-A, Berliner Allee 65, D-86135 Augsburg

Ultrasonic Spray Pyrolysis is a very promising method to produce metal-oxide coatings and particles, respectively, on an industrial scale. Since the Spray Pyrolysis coating process is determined by a large variety of parameters it has the potential to tailor coatings with differ-ent desired properties. For applications a sufficient adhesion as well as an adequate thermal and mechanical stability is required. Here, we demonstrate that the Ultrasonic Spray Pyrolysis is suitable not only to coat planar substrates but also to coat tubular glass substrates.

Using Spray Pyrolysis, yttria was deposited on both, planar and tubular, substrates. A pre-cursor solution containing yttrium nitrate was disposed using an ultrasonic nebulizer. The nebulised droplets subsequently were transferred into a tubular furnace by means of a carrier gas. Additionally particles which were not deposited on the substrate were collected in a glass-fibre filter at the outlet of the furnace. Experiments using different parameter settings were conducted. The as prepared coatings and particles were characterised by SEM and XRD. It is shown how the morphology and chemical composition is controlled by different settings of the processing parameters of the Spray Pyrolysis.

DS 17.11 Tue 9:30 Poster A

Investigation of Metal-Oxide Diffusion Barriers in fluorescent lamps using XPS Depth Profiling — •Christian Berthold[1], Alexandre Santos Abreu[1], Matthias Knoll[1,2], Armin Konrad[2], Reinhard Tidecks[1], and Siegfried Horn[1] — [1]Universität Augsburg, Institut für Physik, EP II, Universitätsstr. 1, D-86159 Augsburg — [2]OSRAM GmbH, FL/CFL D-A, Berliner Allee 65, D-86135 Augsburg

Mercury reduction in fluorescent lamps has become an important environmental issue recently. The goal is to increase the lamps lifetime and at the same time to reduce the amount of mercury dosed into the lamp. To this end, different metal-oxide coatings used as a diffusion barrier for mercury were examined using photoelectron spectroscopy (XPS). The purpose of the investigations was to establish a mercury depth profile within the diffusion barrier.

By layer-to-layer sputtering the surface sensitivity of XPS allows to determine the amount of mercury relative to an element within the diffusion barrier. From the depth profile the effectiveness of various diffusion barriers was determined. The experimentally obtained depth profiles of the mercury concentration within the coating can be described by Fick's laws with an infinite mercury reservoir as boundary condition. We will present the sample preparation as well as different diffusion profiles gained from miscellaneous metal-oxide layers.

DS 17.12 Tue 9:30 Poster A

High-Resolution Depth Profiling of thin high-k layers by means of HRBS — •Maik Vieluf[1,2], Rainer Grötzschel[1], Christian Neelmeijer[1], Marcel Kosmata[1], and Steffen Teichert[2] — [1]Forschungszentrum Dresden-Rossendorf, Deutschland — [2]Qimonda Dresden, Deutschland

The increasing interest in new high-k materials in MOS technology enforces the development of new analytical techniques to characterize the depth dependent elemental composition in ultrathin layers of such materials. The well established methods of ion beam materials analysis as Rutherford Backscattering Spectrometry (RBS) and Elastic Recoil Spectrometry (ERDA) can also provide depth profiles of elements and isotopes with subnanometer depth resolution. These techniques base upon the binary elastic nuclear scattering with well known cross sections and are therefore absolutely quantitative and standard-free. The high energy resolution necessary for high depth resolution is achieved using magnetic spectrometers. We have installed a magnetic spectrometer of the Browne-Buechner-type at the 3 MV Tandetron accelerator of the FZD, which can provide a wide variety of MeV ions both for RBS and for ERDA. To minimise deterioration of the layers due to electronic sputtering during the measurements we implemented a multi-pad position sensitive detector (PSD) in the experimental setup to increase the solid angle and reduce the measurement time. This type of detector gives also the information needed for kinematical corrections. In this poster we describe the high-resolution spectrometer with the improved detector system and show the recent results.

DS 17.13 Tue 9:30 Poster A

Chemical composition of annealed Fe/$SrTiO_3$(001) and FeO/$SrTiO_3$(001) interfaces — •Alexander Demund, Benjamin Heinrich, Rüdiger Szargan, and Reinhard Denecke — Wilhelm-Ostwald-Institut für Physikalische und Theoretische Chemie, Universität Leipzig, Linnéstrasse 2, 04103 Leipzig

Physical interface properties, such as electron and ion conductivity, are strongly tied to the chemical composition of the interfaces. In order to understand processes during deposition or annealing, such as displacement and chemical reactions of atoms in the vicinity of the interface, we have chosen to investigate Fe/$SrTiO_3$(001) and FeO/$SrTiO_3$(001) interfaces by means of chemical state sensitive X-ray photoelectron spectroscopy.

During deposition of Fe in ultra high vacuum at room temperature oxidation of iron and reduction of titanium occurred. Annealing of iron and iron(II) oxide on $SrTiO_3$ caused an inversion of the reaction tendency observed during deposition: iron oxide was in general reduced, while reduced titanium was oxidized. As annealing of $SrTiO_3$ leads to an increasing number of defects, such as oxygen vacancies or Ti(III)-oxygen complexes, we used two differently pre-annealed $SrTiO_3$ crystals (600°C and 800°C). Thermally activated interface reactions occurred at lower temperatures for the crystal pre-annealed at 800°C. On this sample, the number of additional crystal defects detected during annealing was particularly elevated. The increased ion conductivity may play a decisive role in the reactivity of the interfaces.

Work has been supported by DFG (FG 404 Sz58/15).

DS 17.14 Tue 9:30 Poster A

Optical and structural analyses of evaporated thin films of Ga_2Se_3 and In_2Se_3 for solar cells — •Raik Hesse, Raquel Caballero, Daniel Abou-Ras, Christian A. Kaufmann, Thomas Unold, and Hans-Werner Schock — Hahn-Meitner-Institut, Glienicker Str. 100, 14109 Berlin

Ga_2Se_3 and In2Se_3 are used as precursor layers for Cu(In,Ga)Se_2 thin films, which are applied as solar absorbers for photovoltaics. These precursor layers were deposited at various substrate temperatures ranging from 250°C to 450°C on pure glass substrates and on Mo-coated glass substrates. The composition and thickness of the Ga_2Se_3 and In2Se_3 layers can be controlled in-situ by laser (LLS) and white light scattering (WLS). Controlling these parameters is essential since they affect the electrical properties of the Cu(In,Ga)Se_2 layer and therefore the performance of the solar cell. The samples were analysed by optical transmission and reflection measurements in order to determine refractive indexes and band-gap energies complementary to the LLS and WLS results. Ga_2Se_3 and In_2Se_3 were also studied by means of X-ray diffraction (XRD), scanning and transmission electron microscopy, energy dispersive x-ray spectroscopy and grazing-incidence XRD in order to identify different phases and interdiffusion. The formation of a $(Ga,In)_2Se_3$ solid solution was detected and analysed.

DS 17.15 Tue 9:30 Poster A

Microstructure and texture of Nb/$SmCo_5$ bilayers — •Rolf Schaarschuch[1], Silvia Haindl[2], Marianne Reibold[1], Volker Neu[2], Bernhard Holzapfel[2], Carl-Georg Oertel[1], Ludwig Schultz[2], and Werner Skrotzki[1] — [1]Institute of Structural Physics, Dresden University of Technology, D-01062 Dresden, Germany — [2]Institute for Metallic Materials, IFW Dresden, P.O. Box 270116, D-01171 Dresden, Germany

Since the possibility of "magnetic pinning"of vortices was reported many attempts were made to join the obvious antagonistic couple in the form of multilayers with a certain superconductor/ferromagnet sequence. Magnetic pinning describes the interaction between vortices of a superconductor with domain walls of a ferromagnet situated directly above or below the superconductor. Thin film architectures of $SmCo_5$ on Nb and the reversed system both, with and without Cr-spacer layer between superconductor and ferromagnet, were fabricated by pulsed laser deposition. The microstructures and textures/epitaxial relationships of the grown films were characterized by TEM and X-ray diffraction, respectively. As a result, for the layer system Nb/$SmCo_5$ the epitaxial relationship MgO(001)[100]//Cr(001)[110]//Nb(001)[110]//Cr(001)[110]//$SmCo_5$(11-20)[0001]//Cr(001)[110] were found. With decreasing thickness of the Cr-spacer layer the $SmCo_5$ texture becomes random. In contrast, for the system $SmCo_5$/Nb with decreasing thickness of the Cr-spacer layer the Nb texture changes from the component given above to a ¡110¿fibre. The findings are discussed with regard to lattice matching.

DS 17.16 Tue 9:30 Poster A

X-ray Absorption Spectroscopy on La0.7Ce0.3MnO3 films: a critical view on valencies — •Christoph Raisch[1], Mathias Nagel[1], Heiko Peisert[1], Thomas Chassé[1], Robert Werner[2], Dieter Koelle[2], and Reinhold Kleiner[2] — [1]Universität Tübingen, Institut für Physikalische Chemie — [2]Universität Tübingen, Physikalisches Institut - Experimentalphysik II, 72076 Tübingen, Germany

Strongly correlated electrons, lattice distortions and ordering phenomena lead to a highly interesting interplay between spin, charge and orbital degrees of freedom in the doped perovskite manganites $R_{1-x}A_xMnO_3$. Here we report on temperature-dependent XAS and PES measurements on $La_{0.7}Ce_{0.3}MnO_3$ films with varying oxygen content grown by PLD on $SrTiO_3$. The measurements were in part performed at the soft x-ray beamline WERA at ANKA in surface sensitive total electron yield (TEY) and bulk sensitive fluorescence yield (FY) mode. We studied the O K, the Mn $L_{2,3}$ and the Ce $M_{4,5}$ edges, both above and below T_C. Significant differences were found between TEY and FY modes even after thorough self-absorption correction. While the surface signal consists solely of tetravalent cerium and a mixture of di- and trivalent manganese, the fluorescence yield measurements show quite some amount of Ce^{3+} and only minor amounts of the Mn^{2+} species. The valency of manganese is directly related to the kind of doping, electrons or holes, and thus the properties of the sample. The films were further examined with PES of the valence band region and the manganese states. The results are discussed with regard to valency and oxygen content.

DS 17.17 Tue 9:30 Poster A

FT-IR Analyis of supercritical $Si_{1-x}C_x$ alloys — •Ina Ostermay[1], Thorsten Kammler[2], and Torsten Fahr[2] — [1]Fraunhofer Center Nanoelectronic Technologies, Königsbrücker Str. 180, D-01099 Dresden — [2]AMD Saxony LLC & Co. KG, Wilschdorfer Landstraße 101, D-01109 Dresden

Channel strain engineering by the use of lattice-mismatched Source and Drain stressors is widely investigated to improve the carrier mobility in CMOS Technology. In order to increase the performance of N-channel Transistors, embedded layers of Silicon Carbon can be used. Most challenging is the requirement that Carbon atoms need to be present on thermodynamic unstable lattice sites in order to create strain. Since the lattice mismatch at the crystal interface is responsible for the strain generation, the Carbon content needs to exceed the solid solubility limit by several orders of magnitude. For this study, $Si_{1-x}C_x$ layers up to 4,6 % Carbon were grown by Solid Phase Epitaxy (SPE) or Ultra High Vacuum Chemical Vapor Deposition (UHV-CVD) and characterized using SIMS, XRD and Fourier transformation infrared spectroscopy (FT-IR). Carbon was found not to be 100 % incorporated on lattice sites. FTIR was utilized to characterize the phase composition of those metastable layers whereas characteristic vibration modes were observed. These absorption bands could be correlated to the presence of substitutional carbon, coherent precipitates and incoherent 3C-SiC precipitates, respectively. It was found that $Si_{1-x}C_x$ layers created by SPE form incoherent precipitates while epitaxial grown $Si_{1-x}C_x$ alloys tend to form coherent ones.

DS 17.18 Tue 9:30 Poster A

Hard X-ray Photoemission Investigations on Multilayer Coatings for X-ray Optical Devices — •Mihaela Gorgoi[1], Franz Schäfers[1], Christine Borel[2], and Walter Braun[1] — [1]BESSY GmbH, Berlin, Germany — [2]ESRF, Grenoble, France

Many important properties of thin films are determined by the unique features of the interface atoms. A non-destructive way of accessing the electronic properties of buried interfaces is employing high kinetic energy photoelectron spectroscopy (HIKE). State-of-the art Mo/Si multilayers to be used for EUV-lithography and polarisation analysis were investigated by means of HIKE. The measurements were performed at BESSY at the KMC-1 beamline employing the HIKE end-station. A specific example refers to the Mo/Si sample that has a multilayer repetition spacing of d=2.52 nm. To modify the interfacial quality of the multilayers, the samples were heated to a preset temperature, and then subsequently cooled to room temperature, at which time the spectra were taken. The recorded data for 2010 eV excitation energy show different energy shifts occurring in the energy position of the Mo 3d and Si 1s, 2p core levels. Similar behaviour is found at a different probing depth given by 6 keV excitation energy. These results will be correlated with ex-situ x-ray reflectivity measurements performed on the sample before and after the annealing process. A correspondence between the structural changes occurring in the sample and the quality of the interfaces reflected in the electronic properties is pursued.

DS 17.19 Tue 9:30 Poster A

Si nanocrystals in amorphous silica: atomistic models of the interface — •Flyura Djurabekova and Kai Nordlund — Univer-

sity of Helsinki

The poor optical properties of silicon due to its indirect bandgap have until now limited its application in optoelectronics. A novel nanocrystalline approach has disclosed a new prospect for silicon in this field. The observed superior light emitting properties (compared also to porous silicon) of silicon nanocrystals (Si-nc) embedded into amorphous silica (a-SiO_2) are associated with more stable Si/a-SiO_2 interfaces in the new structures. However, the mechanism of this phenomenon still remains unclear. The active role of Si-nanocrystal interface for the optical properties has been discussed intensively. In the present work, we report the creation of atomistic models of the interface by means of molecular dynamics atomistic simulations. Small Si-nc embedded into defect-free a-SiO_2 are constructed using two different classical interatomic potentials. After series of annealing runs, the interface structure and defects are carefully analyzed. The results show a thin suboxide layer along with mostly undercoordinated defects at the interface region.

DS 17.20 Tue 9:30 Poster A

Ion-beam assisted deposition of textured transition metal nitride films — •Martin Kidszun, Ruben Hühne, Konrad Güth, Bernhard Holzapfel, and Ludwig Schultz — IFW Dresden, Institute for Metallic Materials, P.O. Box 270116, D-01171 Dresden, Germany

Ion-beam assisted deposition (IBAD) offers the opportunity to prepare thin textured films on amorphous or non-textured substrates. It was shown within the last decade that thin cube textured layers of materials with a rocksalt structure like MgO or TiN can be produced on amorphous seed layers using this technique. In general, a reactive IBAD process using pulsed laser deposition of transition metals in combination with a nitrogen-containing ion beam was used for the preparation of different transition metal nitride layers. The results on the in-plane textured growth of TiN are promising for the development of conducting buffer layer architectures for YBCO coated conductors based on the IBAD approach. Recent results on the realisation of such an architecture using different substrates as Si/Si_3N_4 or polished Hastelloy tapes will be presented. Furthermore, this approach was used to prepare textured superconducting transition metal nitride thin films as for instance NbN. Detailed measurement of the structural and superconducting properties of such layers will be presented.

DS 17.21 Tue 9:30 Poster A

Low-energy ion beam smoothing of Si surfaces — •Frank Frost, Bashkim Ziberi, and Bernd Rauschenbach — Leibniz-Institut für Oberflächenmodifizierung e. V.

In addition to nanostructuring of various surfaces via self-organized pattern formation, low-energy ion beam erosion can be used as an alternative process for surface smoothing and the preparation of ultrasmooth surfaces. In this work, the surface smoothing of Si surfaces by Ar^+ ion beams (ion energy $\leq$ 2000 eV) was analyzed. Atomic force microscopy (AFM) has been used to systematically investigate the topography evolution of the surfaces with respect to different process parameters. The surface roughness was quantitatively characterized by the first order (rms roughness) and second order (power spectral density - PSD) statistical quantities. Based on the time evolution of these roughness parameters the relevant surface relaxation mechanisms responsible for surface smoothing have been discussed. Especially, it is shown that (i) smoothing can dominate for normal and near-normal ion incidence, (ii) if smoothing occurs, the minimum achievable surface roughness is limited by atomic noise, (iii) for low-energy Ar^+ ion beam erosion of Si surfaces ballistic drift (atomic transport parallel to surface) and ballistic diffusion are the dominant relaxation mechanisms, (iv) secondary sputter effects caused by backscattered projectile ions and sputtered Si atoms have a great impact on the topography evolution, and (v) smoothing by atomic ballistic drift is the most efficient smoothing process at short lateral length scales at normal and near normal ion incidence, respectively.

DS 17.22 Tue 9:30 Poster A

Carbon-Metal-Nanocomposites: Self-organization of multilayers during the co-deposition of energetic ions — •Hayo Zutz[1], Dominika Lyzwa[1], Inga Gerhards[1], Carsten Ronning[1], Michael Seibt[2], and Hans Hofsäss[1] — [1]II. Physikalisches Institut, Universität Göttingen, Friedich-Hund-Platz 1, 37077 Göttingen — [2]IV. Physikalisches Institut, Universität Göttingen, Friedich-Hund-Platz 1, 37077 Göttingen

Thin film growth of metal-carbon compounds by simultaneously low energy deposition of carbon and Fe, Au, Cu or Ni ions reveals a self-organization process resulting in alternating metal-rich and metal deficient layers with layer periods of about 10-20nm. The metal rich layer consists of crystalline clusters >5nm in diameter in an amorphous carbon matrix while the metal-deficient ones of a-C with homogenous distributed metal atoms or small clusters <2nm diameter. The self-organization process occurs only in a certain parameter regime for ion energies and C^+/metal$^+$ fluence ratios. By proper selection of the ratio it is possible to deposit metal-carbon nanocomposite films with homogenously distributed metal clusters (<2nm) in an a-C matrix . We investigated the metal-carbon nanocomposites for the simultaneous depositon of C^+ and Ni^+, Cu^+. The films were analyzed by Rutherford backscattering spectroscopy (RBS), energy dispersive X-ray (EDX) and cross-section transmission electron microscopy (TEM). The results are in agreement with a model for multilayer formation based on an interplay of sputtering, surface segregation, ion induced diffusion and the stability of small clusters against ion bombardment.

DS 17.23 Tue 9:30 Poster A

Formation and superconducting properties of $YBa_2Cu_3O_{7-x}$ / $Y_2Ba_4CuMO_y$ (M=Zr,Nb) quasi-multilayers prepared by off-axis PLD — •Elke Backen, Ruben Hühne, Ludwig Schultz, and Bernhard Holzapfel — IFW Dresden, P.O. Box 270116, 01171 Dresden, Germany

A significant enhancement of pinning forces in YBCO is possible by the introduction of nanosized transition metal particles (Ir, Ti, Hf, Zr) as artificial pinning centres using a quasi-multilayer deposition technique, i.e. the deposition of multilayers of subsequent complete YBCO and incomplete dopant layers. Another promising candidate for the use as artificial pinning centres in YBCO is $Y_2Ba_4CuMO_y$ (Y2411) (M=U, Nb, Ta, W, M, Zr, Ag). These second-phase, nanoscale inclusions have been successfully introduced into large, single-grain, bulk [Rare-Earth (RE)]-Ba-Cu-O superconductors where they form effective magnetic flux pinning sites over a wide range of external magnetic fields. A significant improvement of the J_c and the irreversibility field H_{irr} was observed in these samples. In this work we present first results on YBCO/Y2411 (M=Zr,Nb) quasi-multilayers prepared by off-axis pulsed laser deposition (PLD).

DS 17.24 Tue 9:30 Poster A

Microstructure and self-organization of nano-engineered artificial pinning centers in $YBa_2Cu_3O_{7-\delta}$ coated conductors — •Thomas Thersleff, Elke Backen, Sebastian Engel, Bernd Rellinghaus, Ludwig Schultz, and Bernhard Holzapfel — IFW Dresden, P.O. Box 270116, D-01171 Dresden, Germany

The fabrication of $YBa_2Cu_3O_{7-\delta}$ (YBCO) coated conductors capable of transporting large currents in high external magnetic fields is critical for their commercial implementation. The introduction of nanosized Artificial Pinning Centers (APCs) immobilizes flux lines at higher fields, thus increasing the usefulness and commercial applicability of coated conductors. Moreover, careful nano-engineering of these APCs facilitates the fine-tuning of the superconducting properties of coated conductors such as enhanced pinning along specific crystallographic orientations or an overall reduction in anisotropy. Understanding the self-organizational behavior of these APCs and their effect on the superconducting properties of YBCO thin films is the focus of this work. TEM lamellae from samples prepared on single crystal $SrTiO_3$ using both Pulsed Laser Deposition (PLD) and Chemical Solution Deposition (CSD) methods incorporating APCs were produced using a Carl Zeiss 1540XB Focused Ion Beam (FIB) employing the in-situ lift-out method. TEM investigations on both a FEI Tecnai G^2 and Titan were carried out to elucidate the effect of the processing parameters on the organizational behavior of APCs and to subsequently correlate this to the macroscopic properties of these films.

DS 17.25 Tue 9:30 Poster A

Switchable electro-optical properties of polymer/metal nanocomposites containing chromophores — •Christian Hanisch[1], Christina Pakula[1], Claudia Bornholdt[2], Vladimir Zaporojtchenko[1], Rainer Herges[2], Thomas Strunskus[1], and Franz Faupel[1] — [1]Lehrstuhl für Materialverbunde, Institut für Materialwissenschaft, Technische Fakultät der CAU Kiel, Kaiserstraße 2, 24143 Kiel — [2]Otto Diels-Institut für Organische Chemie (Sektion Chemie), CAU Kiel, Otto-Hahn-Platz 4, 24118 Kiel

It is known that the combination of photoswitchable chromophores like azobenzole with different polymers can be achieved in various ways.

Our aim is to use the photoinduced change in the chromophore conformation in combination with metal/polymer nanocomposites to develop light switchable resistors, optical filters, Bragg-reflectors, capacitors, or other devices. For the sample preparation we used thermal evaporation from up to three independent sources as well as spin-coating of polymers to produce the different sample morphologies needed. The sample morphology was characterized by TEM microscopy. First results with a focus on the tunable electrical resistances in quasi 2D- and 3D- sample geometries are presented.

DS 17.26 Tue 9:30 Poster A

Nano-hole filling with Iron oxides by Atomic Layer Deposition (ALD) — Christian Pfahler[1], •Marc Saitner[1], Alfred Plettl[1], Paul Ziemann[1], Johannes Bikupek[2], Jens Leschner[2], Ute Kaiser[2], Julien Bachmann[3], Yuen Tung Chong[3], and Kornelius Nielsch[3] — [1]Institut für Festkörperphysik, Universität Ulm, D-89069 Ulm, Germany — [2]Materialwissenschaftliche Elektronenmikroskopie, Universität Ulm, D-89069 Ulm, Germany — [3]Institut für Angewandte Physik, Universität Hamburg, D-20355 Hamburg, Germany

Well-ordered periodic nanomasks are generated by a micellar technique [1] and are subsequently used for the preparation of ordered arrays of nanopores. For this purpose a CF_4/CHF_3-gas mixture is applied for etching of Si [2]. The order of the masks is transferred to arrays of pores with diameters between 20 and 30 nm and aspect ratios up to about 10.

After cleaning the substrates by heating in vacuum, the holes are filled with Fe_2O_3 by ALD at 200 °C using ferrocene and ozone as precursors. The Fe_2O_3 filling can be reduced to Fe_3O_4 for further magnetic studies.

The samples are mainly characterized by high resolution scanning (HRSEM) and high resolution transmission electron microscopy (HRTEM) revealing the three dimensional structure.

[1] G. Kästle et al., Adv. Funct. Mat. 13, 853 (2003).

[2] S. Brieger et al., Nanotechnology 17, 4991 (2006).

DS 17.27 Tue 9:30 Poster A

Eigenschaften von Sol-Gel-Aluminiumoxidschichten mit inkorporierten Wolframdisulfid-Nanopartikeln — •Hilke Hattermann, Michael Griepentrog, Marko Szuggars und Thomas Hübert — Bundesanstalt für Materialforschung und -prüfung (BAM), Berlin, Deutschland

Dünne Schichten aus Aluminiumoxid finden bereits seit geraumer Zeit als Verschleißschutzschichten Verwendung, beispielsweise auf Werkzeugen. Durch die Inkorporation von Schmierstoff-Nanopartikeln wie Wolframdisulfid in Form von anorganischen Fullerenen in die Aluminiumoxidschicht wird nun zusätzlich eine Verbesserung des tribologischen Verhaltens erwartet, insbesondere eine Reduktion der Reibung. Das Einbringen der Nanopartikel und die Schichtherstellung erfolgen mit Hilfe eines Sol-Gel-Verfahrens. Die mechanischen Eigenschaften der resultierenden Nanokompositschicht wie Härte und E-Modul, die mit Nanoindentation gemessen werden können, sowie Haftfestigkeit und Rauheit sollten dabei gegenüber einer undotierten Schicht möglichst wenig verändert sein.

Diese Untersuchung findet im Rahmen des EU-Projektes FOREMOST statt.

DS 17.28 Tue 9:30 Poster A

Controlling the formation of Nanoparticles for definite growth of Carbon Nanotubes — •Sascha Hermann, Stefan Schulz, and Thomas Gessner — TU Chemnitz, Center for Microtechnologies, Reichenhainer Strasse 70, 09126 Chemnitz, GERMANY

Our interest is the integration of carbon nanotubes (CNT) in electronic devices (IC, NEMS). This carbon material has some outstanding properties making it a promising candidate fulfilling future requirements for integrated circuit devices (ITRS). Among others we try to replace in a first step the vertical Cu- interconnect with CNT-wires. The requirements for this aim are very challenging as one has to achieve high density aligned CNT-growth with high conductivity at low temperature consistent with microelectronic processes lines (<450°C). In the scope of this work we present a study on the preparation of the catalyst Ni-particles from ultrathin films and the synthesis of carbon nanotubes by the chemical vapour deposition method. For the preparation we use a cold wall CVD-reactor especially designed for handling samples up to a size of a 4 inch wafer. We show the influence of temperature and substrate material on particle formation focusing on optimization of size distribution and density. Furthermore, we present MWNTs grown at temperatures even as low as 500°C. The nanotubes were characterized by scanning electron microscopy, transmission electron microscopy, and Raman spectroscopy.

DS 17.29 Tue 9:30 Poster A

Strong Er luminescence at 1533 nm in rapid thermal annealed Si-rich SiO_2 layers co-implanted with Er — •Aloke Kanjilal, Lars Rebohle, Matthias Voelskow, Wolfgang Skorupa, and Manfred Helm — Institute of Ion Beam Physics and Materials Research, Forschungszentrum Rossendorf, PO Box 51 01 19, 01314 Dresden, Germany

The Er-doped SiO_2 layers containing Si nanocrystals (Si-ncs) have attracted considerable interest for a decade in realizing efficient light sources at about 1540 nm, which coincides with the telecommunication wavelength. Although about two orders of magnitude Er luminescence has been noticed in long time annealed sputtered deposited samples, observation of such high efficiency in ion implantation processed samples is scarce in literature. Recently, we have succeeded in producing such a system by a combination of sequential Si and Er implantations and rapid thermal annealing. The processing conditions have been optimized for achieving maximum Er photoluminescence (PL) at 1533 nm at the expense of the Si-nc related PL band peaking at 870 nm according to the quantum confinement (QC) model, taking the advantage of the visible-range pumping of Er ions by Si-ncs. Spectral analyses suggest that the appearance of a broad PL band at 870 nm can be explained in the light of the interfacial state mediated recombination of carriers in the Si-ncs according to the QC model. The energy migration from Si-ncs to the nearby Er ions has further been manifested using time-resolved PL measurements.

DS 17.30 Tue 9:30 Poster A

Nanostrukturierte Goldfilme als breitbandige Terahertz-Antireflexschicht — •Andreas Thoman, Andreas Kern, Hanspeter Helm und Markus Walther — Freiburger Materialforschungszentrum, Stefan-Meier-Straße 21, 79104 Freiburg

Mit Hilfe der Terahertz Time-Domain Spektroskopie (THz-TDS) [1] wurden die Eigenschaften von nanostrukturierten Goldfilmen auf Silizium im Frequenzbereich von 200 GHz - 2 THz (7 - 66 cm^{-1}) untersucht. Wir zeigen sowohl experimentell als auch theoretisch, dass solche Goldfilme aufgrund ihrer Nanostruktur charakteristische dielektrische Eigenschaften aufweisen, welche es ermöglichen breitbandige Antireflexschichten im THz-Frequenzbereich herzustellen, deren Qualität die homogener Metallfilme [2] übertrifft. Bei optimal gewählter Schichtdicke und Leitfähigkeit des Goldfilms ist es aufgrund Oberflächenimpedanzanpassung möglich, die Reflexion des THz Pulses am Silizium-Gold-Luft Übergang zu unterdrücken. Dieses Verhalten kann mit Hilfe der Finite Difference Time-Domain Methode (FDTD) simuliert werden [3]. Kürzlich konnte gezeigt werden [4], dass die dielektrischen Eigenschaften solcher Filme durch ein modifiziertes Drude Modell (Drude-Smith) beschrieben werden können. Wir zeigen, dass gerade die Abweichung vom idealen Drude-Verhalten die Realisierung einer nahezu perfekten, breitbandigen Antireflexschicht ermöglicht.

[1] P. Uhd Jepsen, A. Thoman et al, Phys. Rev. B 74, 205103 (2006), [2] J. Kröll et al, Optics Express 15 (11), 6552 (2007), [3] A. Kern and M. Walther, J. Opt. Soc. Am. B, submitted, [4] M. Walther et al, Phys. Rev. B 76, 125408 (2007)

DS 17.31 Tue 9:30 Poster A

Sputter deposition of $CuS_{1-x}O_x$ thin films using ceramic targets — •Swen Graubner, Angelika Polity, Detlef Hofmann, and Bruno K. Meyer — IPI Justus-Liebig-Universität Giessen

The efficiency of CuO solar cells can be estimated up to 30%, although the band gap of CuO is about 0.4 to 1.0eV too large compared to the ideal band gap of about 1.5eV. Substitution of oxygen by sulphur may lead to $CuS_{1-x}O_x$ compounds with reduced band gap and might thus have higher efficiencies. The sputter deposition offers several ways for the preparation of $CuS_{1-x}O_x$ thin films: the most common one is to use a metallic Cu target and reactive gases like H_2S and O_2. An alternative is the usage of a sintered (ceramic) Cu_2S target with O_2 as reactive sputtering gas. We concentrated on the later, which has the potential to provide higher sulphur concentrations in the films. The thin films were sputtered under various conditions of the substrate temperature and process pressure. To analyze the morphology, the films were investigated by x-ray diffraction (XRD) and electron microscopy. Secondary ion mass spectroscopy (SIMS) and energy dispersive x-rays (EDX) gave information about the stoichiometry of the layers. The band gap properties as a function of the sulphur content were deter-

mined by optical absorption measurements, and temperature dependent Hall-effect was measured to determine the carrier concentration and the mobility.

DS 17.32 Tue 9:30 Poster A

The influence of electric fields on the time-resolved luminescence of hybrid organic-inorganic structures — •Jędrzej Szmytkowski[1,3], Jonas Conradt[1], Peter Marek[2], Teodor Silviu Balaban[2,3], and Heinz Kalt[1,3] — [1]Universität Karlsruhe (TH), Institute of Applied Physics, Karlsruhe, Germany — [2]Karlsruhe Institute of Technology (KIT), Forschungszentrum Karlsruhe, Institute of Nanotechnology, Karlsruhe, Germany — [3]Center for Functional Nanostructures (CFN), Karlsruhe, Germany

The understanding of the process of electron transfer from an organic dye to inorganic material, like TiO_2 and ZnO, is crucial for the fabrication of efficient hybrid solar cells. Time resolved luminescence studies within applied external electric fields have been performed for several hybrid organic-inorganic structures. The decay associated spectra (DAS) have been used to analyze the dynamics of the luminescence decay. This method allows us to control the dissociation of excitons at the interface of organic-inorganic bilayers.

DS 17.33 Tue 9:30 Poster A

Thickness-dependency of electroreflectance spectra at titanium oxide films — •Andreas M. Zoll and Roger Thull — Lehrstuhl und Abteilung für Funktionswerkstoffe der Medizin und Zahnheilkunde, Universitätsklinikum Würzburg, Pleicherwall 2, D-97070 Würzburg

Thick titanium oxide films have not only attractive properties like good blood compatibility and good corrosion resistance making them very suitable for medical implants, but also very interesting electro optical properties investigated in this study.

The presented titanium oxide films are deposited using unfiltered arc sputtering technique on polycrystalline titanium surfaces. The film thickness is 50 - 200 nm depending ion the deposition time. Substrate temperature was kept at 300 °C.

While thin films of approx. 50 nm showed typical features of low-field electroreflectance spectra at transition energies, ER spectra of thicker films showed oscillations in the sub-gap region corresponding to the first derivative of conventional reflectance spectroscopy.

The band gap was determined using photocurrent spectroscopy and was found at 3.05 +/- 0.05 eV for all samples.

DS 17.34 Tue 9:30 Poster A

Subgridding in the FDTD method for simulating the interaction of terahertz radiation with metal — •Andreas Kern, Hanspeter Helm, and Markus Walther — Deptartment of molecular and optical physics, University of Freiburg

Simulating the interaction of electromagnetic terahertz radiation with metals poses difficulties not encountered in the optical regime. Due to a penetration depth small compared to the wavelength, such simulations in the terahertz frequency range require large discretisation volumes with very small grid spacings. To cope with these large scale differences, a novel subgridding scheme was developed that can be used to accurately describe the interaction of long-wavelength radiation with metals while keeping computational costs minimal. Bidirectional coupling between grids allows for the complete integration of refined subdomains into the simulation volume. Implementation in one and two dimensions is demonstrated, and a comparison with theoretical and experimental results is given. Using our technique, we are able to accurately simulate surface-plasmonic effects in terahertz experiments for the first time.

DS 17.35 Tue 9:30 Poster A

INFRARED ELLIPSOMETRY STUDY OF $LaNiO_3/LaAlO_3$ SUPERLATTICES — •Y. Matiks, A.V. Boris, P. Popovich, H.-J. Kim, G. Cristiani, H.-U. Habermeier, and B. Keimer — Max-Planck-Institut für Festkörperforschung, Heisenbergstr. 1, 70569 Stuttgart

The far-IR variable angle spectroscopic ellipsometry, as a power optical technique for the investigation of the dielectric properties of thin films, was used to study electrodynamics of $LaNiO_3/LaAlO_3$ superlattices. These superlattices with different individual layer thickness and number of interfaces were deposited on $SrTiO_3$, $LaSrGaO_4$, $LaSrAlO_4$ substrates by pulsed laser deposition.

We found that an increasing of substrate lattice parameter and a decreasing of individual layer thickness induce the decreasing of the charge carrier density. A decreasing of the thickness of layer to one unit cell leads to the insulator-metal transition in $(LaNiO_3)n/(LaAlO_3)n$ superlattices on $SrTiO_3$ substrate. This metal-insulator transition may be induced by two factors: 1) localization of the electrons in the context of orbital reconstruction at the interfaces; 2) granulating of layers with the thickness close to one unit cell due to the roughness of substrates.

DS 17.36 Tue 9:30 Poster A

Charge transient spectroscopy (QTS) on organic semiconductors and thin films — •Markus Arnold, Axel Fechner, and Dietrich R.T. Zahn — Physics Department, Chemnitz University of Technology, D-09107 Chemnitz

Charge transient spectroscopy (QTS) is an electrical measurement method related to deep-level transient spectroscopy (DLTS) developed originally by Lang [1]. With DLTS it is possible to investigate charge carrier traps by monitoring capacitance transients. The capacitance is that of the space charge region of inorganic semiconductor or Schottky diodes. Therefore one can not measure samples negligible space charge region using DLTS as is the case for organic semiconductors. The increasing interest in organic semiconductors and organic thin films provides strong motivation for the scientists study the properties of organic devices in depth. With QTS it is possible to measure fast charge reloading processes in the samples as a function of time and the temperature with different pulse voltages and pulse widths. As a result one can determine the number of the traps of e.g. in organic field-effect transistors (OFETs).

[1] D. V. Lang; Deep-level transient spectroscopy: A new method to characterize traps in semiconductors; J. Appl. Phys. 45, 3023 (1974).

DS 17.37 Tue 9:30 Poster A

Kogesputterte Materialien - Einflüsse der Zusammensetzung auf verschiedene Eigenschaften unter Berücksichtigung optischer Funktionalität. — •Christina Polenzky — Fraunhofer-Institut für Schicht- und Oberflächentechnik (IST), Bienroder Weg 54e, 38108 Braunschweig, Deutschland

Ein komplexer Ansatz des optischen Filterdesigns beruht auf einem kontinuierlichen, sinusförmigen Brechzahlprofil, sogenannte Rugate-Filter. Die Vorteile dieses Filter-Typs gegenüber einem herkömmlichen HL-Filter liegen darin, dass es keine scharfen Grenzflächen innerhalb des Schichtsystems gibt, die das thermische und mechanische Verhalten eines optischen Filters stark begrenzen können. In der Praxis lässt sich ein kontinuierliches Brechzahlprofil gut realisieren, indem viele dünne Schichten mit geringen Brechungsindexunterschieden übereinander abgeschieden werden. Diese werden prozesstechnisch meist durch das Mischen zweier Einzelmaterialien in unterschiedlichen Anteilen realisiert. Für das Design des Rugate-Filters wurden bisher, soweit bekannt, nur die optischen Eigenschaften berücksichtigt. In der Anwendung stehen den Vorteilen des Rugates (Wegfall von Grenzflächen) höchste Anforderungen an die Schichtstapel hinsichtlich Haftung und Spannung, auch unter Temperaturbelastung, gegenüber. Beide Eigenschaften sind bei Rugates kritischer als bei konventionellen Filtern, da diese tendenziell aufgrund der geringen optischen Dichte dicker ausfallen.

DS 17.38 Tue 9:30 Poster A

Electromigration in Silver Nanowires — •Christian Wirtz, Niemma Buckanie, Frank-Joachim Meyer zu Heringdorf, and Günter Dumpich — Universität Duisburg-Essen , Fachbereich Physik, Lotharstrasse 1 , 47048 Duisburg

We observe electromigration in silver nanowires by in-situ scanning electron microscopy. Single-crystalline nanowires are prepared employing a self-organised growth process, polycrystalline wires by electron beam lithography (EBL). These nanowires are contacted by voltage and current leads, also using an EBL technique. Electromigration is then induced applying current densities in the range of 10^8 A/cm^2 in either two- or four-terminal mode. Under these conditions, the single-crystalline silver nanowires exhibit a direction of mass flow opposed to that found in their polycrystalline counterparts. This effect is currently believed to originate from surface diffusion effects and to be intimately related to the direct force exerted on the ion cores by the electric field. Further research efforts will comprise investigation of irradiated single-crystals and the role of disorder in electromigration processes. This work is supported by the DFG (SFB 616).

DS 17.39 Tue 9:30 Poster A

Threshold switching in as deposited phase change materials — •Christoph Classen, Michael Woda, and Matthias Wuttig —

I. Physikalisches Institut (1A), RWTH Aachen, 52056 Aachen, Germany

The material class of so called phase change (pc) materials are alloys often containing Sb or Te. Pc materials show an astonishing set of properties as they possess large electrical and optical contrast upon the phase transition from the amorphous to the crystalline phase. On the other hand this reversible transition can be accomplished by either a laser or an electrical pulse on a ns time scale, which makes this material class very promising for memory applications such as PRAM (Phase change RAM).

The threshold switching process is an essential and mandatory feature for phase change material. It enables switching from the amorphous to the crystalline state at low applied voltages and hence is crucial for mobile applications. Presumably this effect is predominantly electronic in nature. In this study our experimental method of choice is presented to measure threshold switching from sputtered as deposited thin films without processing technologically demanding device structures. This approach is employed to investigate the stoichiometry dependence of threshold switching for a number of phase change alloys.

DS 17.40 Tue 9:30 Poster A

Growth of metallic layers on single crystal diamond investigated by infrared spectroscopy — •Sebastian Noebel, Robert Lovrincic, and Annemarie Pucci — Kirchhoff-Institut für Physik der Universität Heidelberg

Electronics based on single crystal diamond provide advantages in many applications, for instance as high energy particle detectors. For all applications the metallization is a decesive step. Besides other metals, chromium and aluminium are often used as electrode materials. Hence we investigate the growth of chromium and aluminium on diamond by means of infrared spectroscopy in order to derive information about the conductivity of the film in a non-contact way. Furthermore, the advantages of the two different metals regarding detector applications will be discussed.

DS 17.41 Tue 9:30 Poster A

Laser deposition of niobium as a refractory metal — •Christian Pansow, Markus Trautmann, Matthias Büenfeld, Veit Grosse, Frank Schmidl, and Paul Seidel — Institut für Festkörperphysik, Jena, Deutschland

Pulsed Laser Deposition (PLD) has become a powerful instrument to grow several types of thin film layers. For some high temperature applications it is essential to use metals with high melting points as conducting materials. In this work, we present the actual state of our studies on the PLD of niobium thin films grown on Si. We investigated the influence of different laser energies, substrate temperatures, argon pressures and energy densities to ensure a high film quality. Our ambition includes good conductivity, low surface roughness, film homogeneity and a low droplet density. We analysed our films with atomic force microscopy (AFM), x-ray diffraction (XRD), auger electron spectroskopy (AES) and scanning electron microscope (SEM).

DS 17.42 Tue 9:30 Poster A

Morphology of ion-beam eroded Si surface: Sputtering at near normal and glancing incident angles — •Kun Zhang[1], Hans Hofsäss[1], Frank Rotter[1], Klaus Jesiek[1], Michael Uhrmacher[1], Carsten Ronning[1], and Johann Krauser[2] — [1]II. Physikalisches Institut and SFB 602, Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany — [2]Fachbereich Automatisierung und Informatik, Hochschule Harz, Friedrichstraße 57-59, D-38855 Wernigerode

Surface morphology evolution induced by ion-sputter-erosion can be explained by a linear continuum theory (developed by Bradley and Harper) of the interplay between ion beam erosion roughening and surface diffusion smoothening processes. This theory predicts the evolution of quasi-periodic surface ripple-patterns, which orientate perpendicular to the beam direction for tilted incidence angles less than a critical angle θ_c (but quite generally, greater than about 30°), or parallel to the beam direction for incidence angles close to grazing. In this work, we report on the evolution of Si surfaces investigated with incidence angles at two extreme cases: near sample normal direction and around the critical angle. The experiments were performed using atomic force microscopy after low-energy (2 – 5 keV) Xe^+ ion irradiation at room temperature with ion-fluences from $3 \cdot 10^{14}$ ions/cm^2 to $1 \cdot 10^{18}$ ions/cm^2. After erosion at near normal direction ($\theta < 30°$), the surfaces are flat and isotropic, in contract to other reports. Two-dimensional nano-patterns evolve after erosion at critical angle θ_c.

DS 17.43 Tue 9:30 Poster A

Modifizierung von Silizium-Oberflächen zur molekularen Erkennung von Peptiden und Proteinen — •Steffen Kröning[1], Karsten Hinrichs[2], Dana Rosu[2], Norbert Esser[2], Jörg Rappich[3] und Rudolf Volkmer[1] — [1]Abteilung Molekulare Bibliotheken, Institut für Medizinische Immunologie, Charité Universitätsmedizin Berlin, Hessische Str. 3-4, 10115 Berlin — [2]Abteilung Interface Spektroskopie, ISAS- Institute for Analytical Sciences, Albert-Einstein-Str. 9 12489 Berlin — [3]Abteilung Silizium-Photovoltaik, Hahn-Meitner-Institut Berlin GmbH, Kekuléstr. 5, 12489 Berlin

Die Untersuchung biologischer Substanzen (z.B. DNA, Proteine, Peptide) gewinnt immer mehr an Bedeutung und ist ein wachsender Bereich innovativer Entwicklungen. Diese Substanzen können durch Sekundärreaktionen (Schlüssel-Schloss-Prinzip) in minimalen Konzentrationen hochspezifisch nachgewiesen werden, wobei vorrangig im ersten Schritt die Bindung an Oberflächen wie Glas, Gold, Cellulose oder Plastik genutzt wird. Durch Kombination von Halbleitertechnik mit organischer Chemie können Oberflächen mit einzigartigen Eigenschaften erzeugt werden. Die Funktionalisierung der Si-Oberfläche mittels ultradünner organischer Schichten und Monolagen von Molekülen wird seit wenigen Jahren intensiver untersucht. Unser Forschungsansatz stellt die direkte Bindung von Linkermolekülen (z.B. Alkenderivate und organische Azidoverbindungen an Si-H terminierten Oberflächen dar. In der gerichteten Immobilisierung dieser Linkermoleküle an Oberfläche besteht die Möglichkeit Peptide und Proteine elektrochemisch mittels einfacher chronoamperometrischer Messungen in Echtzeit zu erkennen.

DS 17.44 Tue 9:30 Poster A

Influence of the process parameters on the photocatalytic activity of TiO_2 thin films deposited by metal plasma immersion ion implantation — •D. Manova[1], F. Haberkorn[1], A. Gjevori[1,2], J.W. Gerlach[1], W. Assmann[3], and S. Mändl[1] — [1]Leibniz-Institut für Oberflächenmodifizierung, Leipzig — [2]Faculty of Natural Sciences, University of Tirana, Tirana, Albania — [3]Ludwig-Maximilians-Universität München, Garching, Germany

Photocatalytic processes have been extensively studied due to their great potential for solvent and air purification and self cleaning. Recently, TiO_2 powder and especially its anatase polymorph attracted a lot of interest as one of the most effective photocatalysts. Metal plasma immersion ion implantation and deposition was employed to form TiO_2 thin films on Si and glass substrates by applying high voltage pulses up to 10 kV in a Ti-O plasma. XRD measurements were performed together with elastic recoil detection analysis (ERDA) to investigate the structure and to derive the stoichiometry, respectively. Additionally, scanning electron microscopy was carried out to investigate the surface morphology. Slightly substoichiometric films with a predominantly rutile structure were obtained. Subsequently, the deposited films were irradiated with UV light. A strong influence of the irradiation on the surface energy of the films, derived from the contact angle measurements, was found with increasing pulse voltage, with an additional influence of the substrate. However, no correlation between the anatase content and the changes in the surface energy was observed.

DS 17.45 Tue 9:30 Poster A

Structural evolution during direct pulsed laser interference patterning — •Stephen Riedel, Matthias Hagner, Paul Leiderer, and Johannes Boneberg — University of Konstanz, Department of Physics, D-78457 Konstanz, Germany

Laser interference lithography with cw-lasers is widely used for the development of micro- and nanostructures on photoresists and subsequent transfer of the structures in the respective substrate. In contrast we present direct laser patterning with a single ns-pulse, where the substrate is structured by several interfering beams. For that purpose we use a frequency doubled Nd:YAG laser (FWHM = 10 ns) and intensities between 50 - 200 mJ. This allows obtaining structured areas of about 1mm^2. We present the energy dependence of structures on different substrates (Au, Ta, Si ...) and show some time resolved measurements on the structuring dynamics. From these measurements a model for the process is developed which is based on Marangoni effects.

DS 17.46 Tue 9:30 Poster A

Pulsed laser deposited $La_{0.7}Ce_{0.3}MnO_3$ thin films: Dependence of properties on growth parameters — •Robert Werner,

Victor Leca, Christoph Back, Reinhold Kleiner, and Dieter Koelle — Universität Tübingen, Physikalisches Institut – Experimentalphysik II, 72076 Tübingen, Germany

$La_{0.7}Ce_{0.3}MnO_3$ thin films were grown epitaxially by pulsed laser deposition on (001) $SrTiO_3$ substrates. The evolution of the growth front and the film thickness were monitored in-situ by means of high-pressure reflection high energy electron diffraction, while the morphology and crystal structure were analyzed by atomic force microscopy and X-ray diffraction, respectively. Furthermore, electrical transport and magnetic properties of the films were studied in the 5–300 K temperature range.
Single phase films could be obtained only for $p_{O_2} > 0.13$mbar. With increasing pressure, the roughness increased. A roughness of one unit cell could only be obtained at a pressure around 3Pa. The evolution of the electric transport and magnetic properties with the level of strain (film thickness) will be discussed. Depending on the deposition parameters we got a transition temperature between 220-260 Kelvin.

DS 17.47 Tue 9:30 Poster A

Magnetic properties and exchange bias effects in nanocluster assembled films of equiatomic Fe-X (X=Pd, Pt, and Au) synthesized by inert gas phase condensation — Chandrahas Bansal[1,2], •Ajay Kumar Mishra[1], and Horst Hahn[1] — [1]Institute for Nanotechnology, Forschungszentrum Karlsruhe, Karlsruhe 76021, Germany — [2]University of Hyderabad, Hyderabad 500 046, India

Nanocluster assembled films of equiatomic Fe-Pd, Fe-Pt, and Fe-Au alloys were synthesized using a UHV nanocluster film deposition system (model NANODEP60 from Oxford Applied Research, UK). The films were nanoporous and consisted of agglomerates of small size nanoclusters of diameters 4 to 5 nanometers. The M(T) data in zero-field-cooled (ZFC) and field-cooled (FC) states revealed a blocking temperature of 33 K, 35K, and 41K for the Fe-Pt, Fe-Pd, and Fe-Au cluster films. Besides this, there was a paramagnetic response at lower temperatures both in the ZFC and FC states showing that there was a partial oxidation of the clusters even in the as-prepared films although they were deposited at base pressures of 10-8 torr. The defect states in the oxide shell gave rise to these moments that remained uncoupled to the antiferromagnetic lattice. A exchange bias of about 1 KOe was observed in all the three alloys with the lowest value for Fe-Au and the highest value for Fe-Pd cluster films.

DS 17.48 Tue 9:30 Poster A

Soft Magnetic nanocomposite films for high frequency applications — •Amit Kulkarni[1], Henry Greve[1], Andreas Gerber[2], Ulrich Schürmann[2], Vladimir Zaporojtchenko[1], Eckhard Quandt[2], and Franz Faupel[1] — [1]Chair for Multicomponent Materials, Institute for Materials Science, Christian-Albrechts University at Kiel, Kaiserstr. 2, Kiel, Germany, 24143. — [2]Chair for Inorganic Functional Materials, Institute for Materials Science, Christian-Albrechts University at Kiel, Kaiserstr. 2, Kiel, Germany, 24143.

Advances in mobile communication have stimulated research on high frequency magnetic components. Nanocomposites with either a particulate or a multilayer nanostructure are promising candidates and could play an important role in such magnetic high frequency applications. Thin multilayer films of sputtered PTFE (Teflon) and $Fe_{54}Ni_{27}Co_{19}$ with different layer thicknesses were prepared by vapor-phase tandem deposition. These films are several hundred nanometers thick and consist of $Fe_{54}Ni_{27}Co_{19}$ as ferromagnetic and a fluoropolymer as the insulating material component. So far we were able to obtain cut-off frequencies up to 5 GHz and HF-permeabilities above 100 for the multilayer nanostructured films. In addition to a Teflon dielectric, FeCoV- TiO_2 / TiO_2 nanocomposite multilayer system were prepared with a very thin isolation layer of TiO_2. Both approaches proved to be promising as novel high frequency components up to the GHz range.

DS 17.49 Tue 9:30 Poster A

Reactive deposition of SnO2:Sb thin films utilizing HPPMS: Correlation between film properties and process parameters — •Janika Boltz, Dominik Köhl, and Matthias Wuttig — I. Physikalisches Institut (1A), RWTH Aachen, 52056 Aachen

In recent years high power pulsed magnetron sputtering (HPPMS) has gained growing interest due to its inherent advantages over conventional dcMS that mainly arise from the increased plasma density and thereby ionization of the sputtered material. It has been demonstrated e.g. for several metal targets that the large degree of ionization (up to 70%) in the sputtered species and the resulting low-energy bombardment of the substrate can promote the growth of films with increased density and low surface roughness. But only recently the new technique has first been applied also to the reactive deposition of metal oxides where e.g. a stabilization of the transition regime has been achieved. In the present work, the potential of HPPMS is explored with respect to the reactive deposition of SnO2:Sb with the aim to develop a comprehensive understanding of the correlations between process parameters and film properties. As a first step, some results of the comparison between dcMS and HPPMS will be shown where both the process characteristics and the film properties are discussed.

DS 17.50 Tue 9:30 Poster A

Atomic layer deposition of silicon dioxide with sub nm-precision — •Robert Zierold[1,2], Julien Bachmann[1,2], Yuen Tung Chong[2], Chris Sturm[3], Marius Grundmann[3], Bernd Rheinländer[3], Ulrich Gösele[2], and Kornelius Nielsch[1] — [1]Institut für Angewandte Physik und Zentrum für Mikrostrukturforschung, Universität Hamburg, Germany — [2]Max-Planck-Institut für Mikrostrukturphysik, Halle/Saale, Germany — [3]Abteilung Halbleiterphysik, Universität Leipzig, Germany

Atomic layer deposition (ALD) is suitable for producing homogenous, thin solid films for various applications in micro- and optoelectronics. We have developed a method for the deposition of silicon dioxide by ALD. Exposure of a flat substrate to consecutive pulses of three gaseous precursors (3-aminopropyltriethoxysilane, water, ozone) deposits SiO2 in monolayer by monolayer fashion. The presence of the amino group within the silane precursor is essential to the growth. It catalyzes the cleavage of the strong Si-O bonds and thereby allows the precursor to bond to the surface.

Electron microscopy, atomic force microscopy and spectroscopic ellipsometry evidence the growth of thin, smooth and pure SiO2 films at a rate of 0.6(+/-0.1) Å per cycle. The novel process allows the conformal deposition of SiO2 into porous alumina templates as well, and yields nanotubes of high aspect ratio (˜1000) with tunable diameter (40 to 160 nm) and wall thickness (1 to 50 nm). We are currently exploring applications to Bragg reflectors, complex optical heterostructures and chemically resistant coatings by this process.

DS 17.51 Tue 9:30 Poster A

Realisation of steady state liquid phase epitaxy for growth of polycrystalline silicon layers on amorphous substrates — •Robert Heimburger, Klaus Böttcher, Thomas Teubner, and Torsten Boeck — Institute for Crystal Growth, Berlin, Germany

The growth of polycrystalline silicon layers on amorphous substrates from metallic solutions at low temperatures is one of the present challenges to overcome the problem of producing low cost thin film solar cells. Generally, the solubility of silicon in metals with low melting point is small at these temperatures.

In order to be able to enhance mass transport of silicon to the surface, we apply a modified classical liquid phase epitaxy called *steady state* liquid phase epitaxy. A detailed experimental study of saturation conditions at the surface of the sample when setting up different heating arrangements will be presented. Selective adjustment of growth and dissolution of silicon at the surface of Si(100) and Si(111) can be shown. Experimental findings will be discussed by means of additional finite-element-simulations of temperature and fluid flow behaviour of the growth arrangement.

DS 17.52 Tue 9:30 Poster A

Reactive Deposition of TiO_x and TiN_x Layers in a DC-Magnetron Discharge — •Stefan Wrehde[1], Marion Quaas[2], Robert Bogdanowicz[3], Hartmut Steffen[4], Harm Wulff[2], and Rainer Hippler[1] — [1]Institute of Physics, University of Greifswald, Felix-Hausdorff-Straße 6, 17489 Greifswald, Germany — [2]Institute of Biochemistry, University of Greifswald, Felix-Hausdorff-Straße 4, 17489 Greifswald, Germany — [3]Department of Optoelectronics and Electronical Systems, Gdansk University of Technology, ul. G. Narutowcza 11/12, 80-952 Gdansk, Poland — [4]Leibnitz-Institute for Plasma Science and Technology e.V., Felix-Hausdorff-Straße 2, 17489 Greifswald, Germany

Thin solid TiO_x and TiN_x films have been deposited by means of a DC magnetron plasma. Reactive gas type (oxygen or nitrogen), reactive gas flow, discharge power and operation mode of the magnetron ("balanced" or "unbalanced") have been varied. Different x-ray techniques (XPS, XR, GIXD) have been applied for research on the chemical composition and the structure of the deposited films. It was found that the operation mode of the magnetron has a significant influence on the

incorporation of oxygen or nitrogen into the layers and also the deposition rate. Comparison of the results of oxygen and nitrogen experiments shows that in unbalanced magnetron mode the incorporation of oxygen into the layers is declined as that of nitrogen is enhanced. By additional application of spectroscopic ellipsometry (SE) the results of the x-ray methods could be confirmed and extended by information on the optical properties of the layers.

DS 17.53 Tue 9:30 Poster A

Production and characterisation of bandwidth- and phase-optimised La/B_4C-multilayer-mirrors for the reflection of ultra short XUV-pulses — •Stefan Hendel, Florian Bienert, Maike Lass, Wiebke Hachmann, Marc D. Sacher, and Ulrich Heinzmann — Department of Physics, Bielefeld University

The applicability of reflective optical components for the XUV region depends upon the existence of multilayer-optics. In particular multilayers for the soft X-Ray spectral range calls for new material combinations. For the photon energy range of about 180 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 3.5 nm (La/B_4C) have been produced by UHV Electron Beam Evaporation combined with Ion Polishing. In-situ layer thickness control is done by X-Ray Reflectometry and single-wavelength Ellipsometry. The characterisation of the layer purity is done by ex-situ Sputter Auger Spectroscopy, whilst structural analysis is performed by X-Ray Diffraction, Transmission Electron Microscopy and at-wavelength reflectivity measurements with Synchrotron radiation. A further goal are aperiodic (chirped) multilayers which exhibit an optimised spectral bandwidth and spectral phase required for the reflection of ultra short soft X-Ray pulses from High Harmonic Sources. We report on experimental results as well as corresponding simulations.

DS 17.54 Tue 9:30 Poster A

Structure formation in reactively sputtered TiO_2 thin films utilizing dcMS and HPPMS deposition techniques — •Azza Amin, Dominik Koehl, and Matthias Wuttig — I. Institute of Physics IA, RWTH Aachen University

TiO_2 thin films are employed in a wide range of applications, e.g. in self-cleaning, antibacterial, antifogging or optical coatings. The as-deposited films usually either possess an amorphous structure or exist in a mixture of the anatase and the rutile phase. The anatase phase is characterized by a pronounced photocatalytic activity, while the rutile structure exhibits a high mass density and a refractive index of up to 2.8 at 2.25 eV. Due to the different physical properties of these two states, a reliable means for the tailoring of the crystalline phase is therefore desirable. The high power pulsed magnetron sputtering (HPPMS) process is expected to be an appropriate tool for this purpose as it facilitates highly ionized deposition due to extremely high peak currents. To develop a thorough understanding of the structure formation and to deposit films with tailored properties, we have performed a comparative study of dcMS and HPPMS deposition processes with the aim of also establishing a detailed description of the correlation between process parameters and film properties. First results of this study are shown.

DS 17.55 Tue 9:30 Poster A

Preparation of single terminated substrates for oxide superlattices — •Thomas Freudenberg, Ruben Hühne, Bernhard Holzapfel, and Ludwig Schultz — IFW Dresden, Institute for Metallic Materials, P.O. Box 270116, D-01171 Dresden, Germany

Well-defined and nearly perfect single crystal surfaces of oxide perovskites are important for the preparation of oxide superlattices with smooth interfaces. Single terminated surfaces of $SrTiO_3$, $NdGaO_3$ and $YAlO_3$ having steps of one unit cell height and atomically flat terraces were obtained by selective etching using various pH controlled hydrofluoric acid solutions. The effect of annealing in an oxygen environment and of etching conditions on the surface morphology was studied by atomic force microscopy (AFM). It has been demonstrated that perfect surfaces can be achieved with a proper selection of both the annealing temperature and the etching parameters with respect to substrate miscut angle. The prepared single terminated substrates were used to study the homoepitaxial growth of $SrTiO_3$ as well as the heteroepitaxial growth of $SrTiO_3$ on $NdGaO_3$ and $SrRuO_3$ on $SrTiO_3$. Therefore, pulsed laser deposition in combination with high-pressure reflection high-energy electron diffraction (RHEED) was applied to investigate the influence of the different deposition parameters including background pressure, substrate temperature and repetition rate on the film growth behavior. The observed RHEED intensity oscillations and the surface characterization using AFM indicate that a layer-by-layer growth mode was achieved during homoepitaxial and heteroepitaxial growth.

DS 17.56 Tue 9:30 Poster A

Metall-PrCaMnO-Heterostrukturen: Struktur und remanente Widerstandsänderungen — •Julia Fladerer, Jörg Hoffmann, Peter Moschkau und Christian Jooss — Institut für Materialphysik, Universität Göttingen

Remanente Widerstandsänderungen in gepulsten elektrischen Feldern an Oxid-Metall Heterostrukturen sind vielversprechende Kandidaten für neue nichtflüchtige Speicher. PCMO Dünnfilme wurden mittels Ionenstrahlsputtern epitaktisch auf (100)-orientierten Pt-Filmen deponiert. Die Schichtdicke betrug ca. 120nm für die Pt- und 330nm für die PCMO-Schicht. Für verschiedene obere Elektrodenmaterialien (Pt, Au, Ag, Cu, Al, ITO) zeigten die Heterostrukturen stark unterschiedliches Verhalten der remanenten Widerstandsänderungen bei Raumtemperatur sowie der Strom-Spannungs-Kennlinien. Die zur Beschreibung der Manganate verwendeten Modelle der thermisch aktivierten Polaronen und der raumladungsbegrenzten Ströme können diese Beobachtungen nicht erklären. Es wird das Modell eines korrelierten Schottky-Kontaktes entwickelt, der Polaronenverhalten mit Bandverbiegung an der Metall-Oxid Grenzfläche verbindet und so qualitative Übereinstimmungen liefert.

DS 17.57 Tue 9:30 Poster A

Preparation of thin biaxial strained functional oxides — •Sascha Trommler, Thomas Freudenberg, Ruben Hühne, Bernhard Holzapfel, and Ludwig Schultz — IFW-Dresden, Germany

In the last years functional oxides with a perovskite structure as well as structurally related compounds have attracted great interest. It had been shown, that between interfaces of such epitaxial oxides novel electronic structures can be formed or that the biaxial strain induced by the lattice mismatch may affect the physical properties significantly in these materials. A main prerequisite to study these effects is the controlled growth of epitaxial heterostructures on an atomic level in order to achieve smooth interfaces with a low density of defects. Therefore, pulsed laser deposition was used in combination with in-situ RHEED observation to prepare such heterostructures on single terminated atomically flat substrates. Results on the layer-by-layer growth of different functional oxides as $SrRuO_3$, $La_{2-x}Ba_xCuO_4$ and of $LaCoO_3$ will be presented and discussed together with their structural and physical properties.

DS 17.58 Tue 9:30 Poster A

Local variation of dispersion constants of ITO films studied by spectroscopic imaging ellipsometry — •Matthias Vaupel[1] and Mykola Vinnichenko[2] — [1]Nanofilm Technologie GmbH, 37081 Göttingen, Germany — [2]Forschungszentrum Dresden-Rossendorf, Institute of Ion Beam Physics and Materials Research, P.O.Box 510119, 01314 Dresden, Germany

Tin-doped-indium oxide (ITO) is a degenerate n-type semiconductor with high transparency and nearly metallic conductivity. Thin films of ITO find applications as transparent electrodes in optoelectronics (including organic light emitting devices (OLEDs)), photovoltaics, and in the liquid crystal display industry. A standard route of producing ITO films is deposition by magnetron sputtering. The interaction of the magnetron plasma with the growing film surface may be employed to cause inhomogeneity of the film morphology [1]. The aim of the present work is to study the influence of the intentionally inhomogeneous plasma flow on the distribution of the ITO film thickness and optical properties (dispersion parameters: free charge density, frequency and force of the Lorentz oscillator, and the constant term) along the substrate. Variation of the film properties are investigated both on large (several milimeters) and local (several micrometers) scale.

[1] A. Rogozin, M. Vinnichenko, N. Shevchenko, A. Kolitsch, and W. Moeller, Thin Solid Films 496, 197 (2006).

DS 17.59 Tue 9:30 Poster A

Electrodeposition of porous ZnO on textile substrates — •Markus Mingebach[1], Thomas Loewenstein[1], Yvonne Zimmermann[2], Andreas Neudeck[2], and Derck Schlettwein[1] — [1]Justus-Liebig-Universität Gießen, Institut für Angewandte Physik, Heinrich-Buff-Ring 16, 35392 Gießen — [2]Textilforschungsinstitut Thüringen-Vogtland e.V., Zeulenrodaer Straße 42, 07973 Greiz

Textile integrated photovoltaic cells are of interest to realize a standalone energy supply of textile electronics which are presently developed for applications in safety and health care. A low temperature deposition method of photovoltaic structures (< 150 °C) is required for textiles. Sensitized ZnO as a wide bandgap semiconductor applied in photoelectrochemical photovoltaic cells [1] can be utilized for this purpose. Such ZnO films can be obtained at 70 °C from aqueous zinc salt solutions by electrochemical deposition. By adding the structure directing agent EosinY to the deposition solution, highly porous films with roughness factors of about 200-400 are prepared [2]. In this study we report the growth of ZnO/EosinY hybrid films on metal coated polyamide threads and filaments. The influence of the deposition parameters like current density and hydrodynamic aspects on the electrode parameters was analyzed by scanning electron microscopy (SEM) and photoelectrochemical experiments.

[1] T. Yoshida, M. Iwaya, H. Ando, T. Oekermann, K. Nonomura, D. Schlettwein, D. Wöhrle, H. Minoura, Chem. Comm., 4, 400 (2004)
[2] T. Yoshida, M. Tochimoto, D. Schlettwein, D. Wöhrle, T. Sugiura, and H. Minoura, Chem. Mater., 11, 2657 (1999)

DS 17.60 Tue 9:30 Poster A

Study of the formation mechanisms of the polycrystalline thin films of GaSb on non-orienting substrates during forced cooling of saturated solution-melt — •Andrey Sarikov[1], Yevgen Baganov[2], and Stanislav Shutov[1,2] — [1]V. Lashkarev Institute of Semiconductor Physics NAS Ukraine, 45 Nauki avenue, Kiev 03028, Ukraine — [2]Kherson National Technical University, 24 Berislavs'ke highway, Kherson 73008, Ukraine

Thin films of crystalline GaSb on inexpensive non-orienting substrates (e. g. glass) are interesting as a basis for the production of low-cost photovoltaic and thermophotovoltaic converters. In this work, we propose a new method of obtaining thin polycrystalline GaSb films on non-orienting substrates based on a forced cooling of saturated solution-melt of Sb in Ga. The morphology of GaSb layers is studied experimentally as a function of annealing and cooling down conditions. A theoretical model of the process under investigation is suggested and the kinetics of the nucleation and growth of GaSb grains during forced cooling of saturated solution-melt is studied theoretically. The appearance of crystalline GaSb grains is found to be due to the heterogeneous nucleation at the interface of amorphous Sb/Ga+Sb solution-melt with the vacuum surrounding. The optimisation procedure for the formation of polycrystalline GaSb films on non-orienting foreign substrates with respect to process duration and final grain size is studied. The process described is also proposed to use for the formation of the polycrystalline thin films of other A3B5 semiconductors on the non-orienting foreign substrates.

DS 17.61 Tue 9:30 Poster A

An in situ GISAX study on the shape anisotropy of sputter grown Ta — •Kai Schlage, Sebastien Couet, Ralf Röhlsberger, Andreas Timmmann, and Stephan Roth — Deutsches Elektronen Synchrotron (DESY), Hamburg, Germany

It is well known that the shape anisotropy of polycrystalline grains in thin films can strongly influence their intrinsic magnetic properties like magnetic hard and easy axes. Also buffer layers contribute to this effect. We use Grazing Incidence Small Angle X-Ray Scattering (GISAXS) to follow in-situ the structural evolution of obliquely sputter deposited Ta onto a Si wafer which is often used as buffer layer in magnetic thin film systems. GISAXS allows to follow the growth process of the films and yields the size, shape and the lateral correlations of surface structures like nanoislands in the initial stage of film growth [1]. We found a strong growth anisotropy of the Ta which can be directly related to the sputtering geometry.

[1] S.V. Roth et al., Applied Physics Letter 88, 021910 (2006)

DS 17.62 Tue 9:30 Poster A

Metal organic chemical vapour deposition of $SrRuO_3$ thin films on $SrTiO_3$ — •Rasuole Dirsyte, Jutta Schwarzkopf, Günter Wagner, and Roberto Fornari — IKZ, Max Born - Straße 2, D - 12489 Berlin, Germany

$SrRuO_3$ with pseudo-cubic crystalline structure (a = 0.393 nm) appears to be one of the most suitable conductive oxides to be used as bottom electrode for the oxide-based electronic devices, due to its high conductivity and low lattice misfit with many functional perovskite transition metal oxides [1]. Furthermore, this electrode has a lower density of defects (oxygen vacancies, dislocations, dead layer) compared with metal electrodes (Pt, Ru, Ir) [2].

A vertical liquid-delivery metal-organic chemical vapour deposition (MO-CVD) reactor was used to deposit (100)-oriented $SrRuO_3$ films on vicinal $SrTiO_3$(100) substrates. In order to grow epitaxial thin films with low defect density and high electrical conductivity and to optimise the deposition parameters, the influence of deposition temperature (500 - 700 °C), argon/oxygen ratio (1,6 - 3,3), total gas flow (4875 - 8125 sccm) and reactor pressure (12 mbar - 40 mbar) was investigated.

Composition of the films was identified by GDOES technique. Raman and XRD were used to determine film orientation and the surface morphology and roughness was analysed by AFM and SEM microscopy.

[1] O. Gautreau, C.Harnagea, F. Normandin, T.Veres, A. Pignolet, Thin Solid Films 515, 4580 (2007).
[2] N. Menou, H. Kuwabara, and H. Funakubo, Jpn. J. Appl. Phys. 46, 2139 (2007).

DS 17.63 Tue 9:30 Poster A

Influence of growth conditions on surface morphology, structural and optical properties of PbSnTe/BaF_2/CaF_2/Si(100) heteroepitaxial structures — •Dmitriy Ostertak[1], Alexander Velichko[1], Vladimir Ilyushin[1], Marion Friedrich[2], and Dietrich R.T. Zahn[2] — [1]Novosibirsk State Technical University, Novosibirsk, Russia — [2]Chemnitz University of Technology, Chemnitz, Germany

Epitaxial films of group II fluoride insulators grown on silicon are used to produce semiconductor-on-insulator structures and buffer layers for heteroepitaxy. Among them, the most promising candidates are Si / CaF_2 / Si and PbSnTe / BaF_2 / CaF_2 / Si structures which are used to manufacture high-speed radiation-resistant very large scale integrated circuits and monolithically integrated photodetector arrays. Most of the published papers are devoted to CaF_2 and BaF_2 epitaxy processes on silicon surfaces with (111) orientation while the (100) orientation is more attractive for solving technical applications mentioned above.

CaF_2 / Si(100), BaF_2 / CaF_2 / Si(100) and PbSnTe/BaF_2 / CaF_2 / Si(100) heteroepitaxial structures were grown by Molecular-Beam Epitaxy at different growing conditions. The surface morphology was investigated by Atomic Force Microscopy (AFM). The optimal growing conditions for CaF_2 on Si(100), BaF_2 on CaF_2 / Si(100), and PbSnTe on BaF_2 / CaF_2 / Si(100) were determined from AFM measurements. Fourier transform infrared spectroscopy and spectroscopic ellipsometry were used to study optical properties and to measure thickness of these films. The influence of different growth conditions on optical and structural properties is discussed.

DS 17.64 Tue 9:30 Poster A

Measurement of the internal mechanical dissipation in dielectric thin films — •Stefanie Kroker[1], Christian Schwarz[1], Daniel Heinert[1], Ronny Nawrodt[1], Anja Schroeter[1], Ralf Neubert[1], Matthias Thürk[1], Sandor Nietzsche[1], Wolfgang Vodel[1], Andreas Tünnermann[2], and Paul Seidel[1] — [1]Institut für Festkörperphysik, Helmholtzweg 5, 07743 Jena, Germany — [2]Institut für Angewandte Physik, Albert-Einstein-Straße 15, 07745 Jena, Germany

Gravitational wave detectors currently under operation are limited by different kinds of noise. One of the fundamental noise sources of future detectors will be thermal noise arising from the dielectric coatings of the optics. In order to fulfil the requirements for the third generation gravitational wave detectors it is necessary to reduce the mechanical dissipation of the dielectric thin films by at least a factor of 2. Thus, it is necessary to understand the internal mechanisms that cause mechanical loss. We present a novel set-up to measure the internal mechanical dissipation of thin films ($< 1\,\mu$m) on silicon substrates. We present results for tantala (Ta_2O_5) and silica (SiO_2) within a temperature range from 5 to 300 K.

This work is supported by the German science foundation under contract SFB Transregio 7.

DS 17.65 Tue 9:30 Poster A

Dielektrische Bragg–Spiegel für Zinkoxid–Mikrokavitäten — •A. Dempewolf, A. Franke, A. Diez, B. Diez, J. Bläsing, T. Hempel, J. Christen und A. Krost — Institut für Experimentelle Physik, Otto-von-Guericke-Universität Magdeburg, Deutschland

Zur Herstellung von ZnO-basierten Mikrokavitäten sowie Polaritonen-Lasern werden qualitativ hochwertige Bragg-Spiegel (DBR) benötigt. Das epitaktische Wachstum dieser auf Grundlage von MgZnO gestaltet sich jedoch schwierig. Eine Alternative bietet die Verwendung von dielektrischen Materialien. Es wurden dielektrische DBRs bestehend aus

$\lambda/4$ – Tantal(V)- und Silizium(IV)oxid-Schichten auf Silizium-Substrat mittels Elektronenstrahlverdampfen abgeschieden. Aufgrund der hohen Brechungsindexdifferenz beider Materialien von 0,6 im Bereich der exzitonischen Lumineszenz von ZnO (I_8 = 3,36 eV) konnten bereits bei 10,5 Schichtpaaren eine Reflektivität von über 99,5 % und eine Weite des Stoppbandes von 540 meV erreicht werden. Vergleichend dazu erfolgte die Herstellung der DBRs basierend auf den hochbrechenden Materialien Hafnium(IV)- und Zirkon(IV)oxid. In einem weiteren Schritt wurden auf einen 10,5 - paarigen unteren Spiegel eine 3 $\lambda/2$–Silizium(IV)oxid-Kavität und ein 10 - paariger oberer Spiegel abgeschieden. Das Reflexionsspektrum weist eine Kavitätsmode bei 3,28 eV mit einem Q-Faktor von 130 auf. Ein effizientes optisches Pumpen der aktiven Zone wird durch eine hohe Transmission im Bereich der HeCd-Laserlinie bei 3,81 eV ermöglicht. Zum Erzielen einer starken Licht-Materie-Kopplung wurde eine gesputterte ZnO-Schicht als aktives Medium in die Struktur integriert.

Another 12 posters from High-k Dielectric Materials - Synthesis, Properties, Applications, for abstracts look on Wednesday 18:30 - 20:30

DS 18: Poster: Towards Molecular Spintronics, Organic Thin Films, Optical Layers, Vibrational Spectroscopy, Tayloring organic interfaces

Time: Tuesday 14:30–19:30 Location: Poster A

DS 18.1 Tue 14:30 Poster A

Stability and spin coherence of hydrogen atoms trapped in pure silica zeolite — •Rolf Simon Schoenfeld[1], Wolfgang Harneit[1], and Corma Avelino[2] — [1]Institut für Experimentalphysik, Freie Universität Berlin, Arnimallee 14, D-14195 Berlin, Germany — [2]Instituto de Tecnología Química UPV-CSIC, Universidad Politécnica de Valencia, Avenida de los Naranjos s/n, 46022 Valencia, Spain

We report the first observation of electron paramagnetic resonance (EPR) of hydrogen atoms trapped in pure silica LTA zeolite after gamma irradiation of n-hexane filled samples. Heating experiments revealed stability up to 80 °C in both air containing and evacuated samples. The small isotropic line width and the low deviation of hyperfine coupling constant and g-factor from the free atom values indicate a minimal distortion of the electron wave function. In addition, spin lattice and spin spin relaxation times T1 and T2 were measured by means of FT EPR. Although relaxation by spin diffusion cannot be excluded, a long spin coherence time of more than 12 microseconds was observed at ambient temperature in an evacuated sample.

DS 18.2 Tue 14:30 Poster A

Observation of spin switching in a chainlike supramolecular Fe (II) complex observed by STM/CITS — •M. Stocker[1], A. Volkov[1], M.S. Alam[1], V. Dremov[1], M. Ruben[2], and P. Müller[1] — [1]Institut für Physik der Kondensierten Materie, Universität Erlangen-Nürnberg — [2]Institut für Nanotechnologie, FZ Karlsruhe

Using a home-made microscope and custom-build control electronics and software we performed STM/CITS measurements on a chainlike supramolecular Fe (II) complex. The investigated complex shows spin crossover from a low-spin to a high-spin state in a temperature range between 250-350K. We investigated single and multiple polymer strands deposited onto HOPG surfaces. STM topography was able to resolve single monomers. The CITS technique at ambient conditions showed two distinct monomer species, one highly conducting, the other close to insulating. Furthermore we were able to observe spontaneous reversible switching between the two states. The different conductance can be attributed to the different spin states of the Fe (II) metal center. We discuss the results in terms of spin crossover theories.

DS 18.3 Tue 14:30 Poster A

Magnetization Tunneling and Quantum Transport in Single Molecule Magnets — •Nikolaos P. Konstantinidis[1,2], Maarten R. Wegewijs[1,2], Christian Romeike[1], Herbert Schoeller[1], and Walter Hofstetter[3] — [1]Institut für Festkörper-Forschung - Theorie III, Forschungszentrum Jülich, 52425 Jülich, Germany — [2]Institut für Theoretische Physik A, RWTH Aachen, 52056 Aachen, Germany — [3]Institut für Theoretische Physik, J. W. Goethe-Universität, D-60438 Frankfurt, Germany

The electric current through a single molecule magnet is investigated theoretically as function of an external magnetic field. We present results for the linear transport regime obtained by the numerical renormalization group (NRG) technique [1], as well as non-linear transport properties obtained using quantum kinetic equations. We predict effects related to the coherent magnetization tunneling generated by the magnetic anisotropy. In particular, we show how non-trivial Kondo and spin-tunneling effects allow for a complete determination of the magnetic properties of such a device by transport experiments.

[1] M. R. Wegewijs, C. Romeike, H. Schoeller and W. Hofstetter, New J. Phys. 9 344, (2007).

DS 18.4 Tue 14:30 Poster A

Identifying the single-molecule spin states by vibronic transport effects — •Felix Reckermann[1,2], Maarten R. Wegewijs[1,2], and Herbert Schoeller[2] — [1]Institut für Festkörper-Forschung - Theorie 3, Forschungszentrum Jülich, 52425 Jülich, Germany — [2]Institut für Theoretische Physik A, RWTH Aachen, 52056 Aachen, Germany

We show that an electric current through a mixed-valence dimer molecule can detect the spin states of the electronic excitations without external magnetic field. Mixed-valence complexes are molecules in which an excess electron can tunnel between hetero-valent metal ions. This tunneling mediates both a ferromagnetic double-exchange interaction between the ionic spins as well as a non-adiabatic electron-vibration (so called vibronic) interaction.

One has to account for the coupling of the electron motion to the breathing mode of the two ionic ligand-shells as well as the breakdown of the Born-Oppenheimer approximation. The resulting entanglement of the electronic and vibrational degrees of freedom can be detected by a sharp dependence of the differential conductance on the electromechanical parameters. Furthermore, the double-exchange coupling of the ionic spins and the vibrational motion become correlated. In a three terminal device geometry, this allows one to identify the spin states of the molecule using the FC-effect.

DS 18.5 Tue 14:30 Poster A

On the electronic structure of cobalt phthalocyanine — •Thomas Kroll[1], Victor Yu. Aristov[1,2], Olga V. Molodsova[1], Victor M. Zhilin[2], Denis V. Vyalikh[3], Bernd Büchner[1], 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]Institute of Solid State Physics, TU Dresden, D-01069 Dresden, Germany

Metal phthalocyanines (MPc) are molecular based systems that contain a transition metal ion in its centre. They have long been attractive materials for fundamental aspects as well as technological interest. Furthermore, metal phthalocyanine complexes have the potential to provide important information on general questions regarding metal-organic complexes. They may thus act as archetype model systems for the physical behaviour of a large number of other TM complexes.

In this presentation, we will concentrate on cobalt phthalocyanine (CoPc). In this material, the Co ion appears in a divalent state with formally 7 electrons in the 3d shell. We will show results of spectroscopic measurements such as X-ray absorption spectroscopy at the Co L-edge, together with a theoretical description of the data. This approach has already proved to work successfully for transition metal oxides. Our results will clarify important aspects of the electronic structure of CoPc and shed further light on general questions regarding metal-organic complexes.

DS 18.6 Tue 14:30 Poster A

Electronic excitation spectra of transition metal phthalocyanines — •Roberto Kraus, Mandy Grobosch, and Martin Knupfer — IFW Dresden, D-01069 Dresden, Germany

The electronic structure of transition metal phthalocyanine (TMPc) complexes offer valuable insight into the interaction of the metal ion

with its surrounding, the organic ligand. Therefore, they represent simple model compounds for the investigation of the electronic properties of many other transition containing molecules, among them many molecular magnetic complexes. In fact, MnPc has been referred to as a typical example of a molecular magnet. Surprisingly, despite a large number of experimental and theoretical studies essential details of the electronic structure and excitations of TMPcs remained unclear, but are of tremendous importance to understand the spin and charge ground state of the enclosed transition metal ion. We present a characterization of the full electronic excitation spectra of MnPc and FePc, which have been determined using optical as well as electron energy-loss spectroscopy. We discovered low lying electronic excitations that have been observed in the past and discuss the results in view of previous theoretical work.

DS 18.7 Tue 14:30 Poster A

Growth of CuPc thin films and metal contact formation: A photoemission study — •Teodor Toader[1], Gianina Gavrila[2], Jan Ivanco[1], Walter Braun[2], and Dietrich R.T. Zahn[1] — [1]Department of Physik, Technical University Chemnitz, D-09107 Chemnitz, Germany — [2]BESSY GmbH, Albert-Einstein-Straße 15, D-12489 Berlin, Germany

In this study both organic/inorganic semiconductor and metal/organic film interfaces prepared under ultra-high vacuum conditions will be addressed. The growth of highly-ordered copper phthalocyanine (CuPc) films on stepped Si(111) surfaces was investigated by photoemission and near edge X-ray absorption fine structure (NEXAFS). While the molecules take an upright orientation on hydrogen-passivated surfaces, the passivations by an ultra-thin antimony layer lead to a near lying molecular orientation. The molecular geometry in the CuPc film grown on the hydrogen-Si(111) surface was significantly influenced using a template film of 3,4,9,10-perylenetetracarboxylic dianhydride (PTCDA) deposited prior to CuPc growth. Varying molecular orientation in the CuPc films affects their electronic properties as probed via valence band photoemission spectroscopy. The interfacial chemistry and electronic structure of a metal contact, namely In-CuPc was studied during the incremental overgrowth of indium. A chemical interaction between indium and CuPc film was detected with reacted molecules tending to remain on the In surface, rather than at the In-CuPc interface.

DS 18.8 Tue 14:30 Poster A

Spectroscopic determination of the Voigt constant of copper phthalocyanine by magneto-optical Kerr effect and ellipsometry investigations — •Michael Fronk, Dietrich R.T. Zahn, and Georgeta Salvan — Physics Department, Chemnitz University of technology, D-09107 Chemnitz

The measurement of the magneto-optical Kerr effect (MOKE) is frequently used to monitor magnetic properties of ferromagnetic thin films during growth (e.g. [1]). MOKE spectroscopy can also be employed to determine the Voigt constant of ferromagnetic layers [2,3], if the optical constants of the involved layers are known. In this work the Voigt constant of copper phthalocyanine (CuPc) is calculated using the experimental results of polar MOKE spectroscopy and variable angle spectroscopic ellipsometry (VASE) investigations. The calculations were carried out using a three layer model air - film - substrate for normal incidence and considering the decomposition of the linearly polarised incident light into its two circularly polarised eigenmodes. The CuPc films were grown by organic molecular beam deposition in high vacuum onto silicon substrates either H-passivated or covered by native oxide. When deposited on silicon with native oxide the molecules adopt a close to standing orientation, while those grown on H-passivated substrates align with an average tilt angle of about 55° with respect to the substrate plane. This leads to significant differences in the magnitude of the Voigt constants of CuPc on the two types of substrates.

[1] M. Wahl et al., phys. stat. sol. (c) 0, 2003, 3002 [2] T. Herrmann et al., PRB 73, 2006, 134408 [3] J. Zak et al., PRB 43, 1991, 6423

DS 18.9 Tue 14:30 Poster A

Optically detected magnetic resonance of single N-V centers in diamond for molecular spintronics — •Juliane Kniepert, Kati Hübener, Christoph Oelmüller, and Wolfgang Harneit — Institut für Experimentalphysik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany

An important issue in molecular spintronics is the detection and state read-out of single spins or small spin ensembles as occur in molecular nanostructures. With their typical sensitivity of 10^{12} to 10^{14} spins, conventional ESR methods are not suitable for single spin detection. Optical detection (ODMR) improves the sensitivity to 10^5 spins. Combined with single molecule spectroscopy, the spin of an individual molecule becomes accessible.

Here, we apply the method of single spin detection to N-V centers in diamond as a read-out system for molecular spins. The nitrogen-vacancy (N-V) center consists of a substitutional nitrogen atom and an adjacent carbon vacancy. Irradiation of resonant microwaves changes the spin polarization of the ground state, resulting in a decrease of the fluorescence intensity. N-V centers are also interesting for the field of quantum information. They might be used as qubits themselves or as a read out system for other coupled spin systems e.g. organic molecules. Here we investigate the coupling of endohedral fullerenes to N-V centers. Owing to their long relaxation time endohedral fullerenes such as $N@C_{60}$ may be promising candidates for quantum bits.

DS 18.10 Tue 14:30 Poster A

Optimization of spin coated thin films based on transition metal complexes towards magneto-optical applications — •Björn Bräuer[1], Tobias Rüffer[2], Robert Mothes[2], François Eya'ane Meva[2], and Georgeta Salvan[2] — [1]Chemnitz University of Technology, Department of Physics, Reichenhainer Straße 70, D-09126 Chemnitz — [2]Chemnitz University of Technology, Department of Chemistry, Straße der Nationen 62, D-09111 Chemnitz

Coordination complexes allow the step-wise incorporation of an increasing number of transition metal ions and thereby the variation of physical properties of the molecules. In this work a series of bis(oxamato) type transition metal complexes containing three Cu(II) ions were synthesized to investigate the influence of their central N,N'-bridge and of their terminal ligands on the magnetic and magneto-optical properties. The latter were investigated by means of magneto-optical Kerr effect (MOKE) spectroscopy. For the MOKE investigations thin films were prepared by means of spin coating (deposition) on Si wafers. This was previously demonstrated for the first time to be a promising technique for the deposition of multinuclear transition metal complexes on surfaces [1]. To improve the quality of the films in terms of homogeneity, a number of parameters had to be optimized: a) the chemical composition of the multinuclear transition metal complexes with respect to their planarity and solubility, b) the rotation speed as well as the solvent in the spin coating process. [1] B. Bräuer, D. R. T. Zahn, T. Rüffer, G. Salvan, Chem Phys Lett, 2006, 432, 1-3, 226.

DS 18.11 Tue 14:30 Poster A

All-electron calculations of spin-polarized transport through molecules — •Daniel Wortmann, Nicolae Atodiresei, and Stefan Blügel — Institut für Festkörperforschung, Forschungszentrum Jülich, 52425 Jülich, Germany

The magneto-resistive effects and coupling between an electron current and the magnetisation in planar junctions is a highly developed field and forms the basis of the field of spintronics and magnetoelectronics. The experimental and theoretical studies of related effects in molecular junctions is still at its infancy. We investigate a model system of a magnetic cobaltocene molecule sandwiched between Ni(111) surfaces by carrying out *ab initio* density functional theory (DFT) calculations of the spin-depended transmission. The calculations of electron transport through molecules in linear response became nearly a standard for the popular gold electrodes. Our all-electron full-potential transport code is ideally suited to treat as well more complex materials and relativistic effects as well as non-collinear magnetic structures are included. Support by the DFG-SPP 1243 is gratefully acknowledged.

DS 18.12 Tue 14:30 Poster A

Structure and morphology of thin evaporated Polycarbonate films — •Christian Vree and S. G. Mayr — I. Physikalisches Institut, Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen

Structure formation at surfaces during thin film deposition is of great scientific interest due to the demand for smooth or regularly structured surfaces and interfaces for miniaturized functional films in science and technology. The deposition processes which govern morphology evolution during vapour deposition of polymer films are still poorly understood and need closer investigation.

Poly (Bisphenol A carbonate) (PC) thin films were deposited in a vacuum chamber on different substrates. Surface morphologies were investigated using scanning force (SFM) and scanning electron microscopy (SEM). Fourier transform infrared spectroscopy (FTIR) and

size exclusion chromatography (SEC) were performed for a detailed chemical characterization. It is found, that the bond topology remains mostly unchanged, while the chain length is reduced. Evaporated films basically consist of oligomeric fractions (dimer to heptamer) of the original chains but a small amount of high molecular weight material can be observed as well. The rms-roughness decreases rapidly with film thickness on Si, SiO_2 and GaAs substrates, until a fully covered substrate is obtained at thicknesses as high as 30 nm. On PC substrates smooth films are observed independent of film thickness.

This work is financially supported by the DFG SFB 602 (TP B3), as well as the GIF No. 1428-303.1/2004.

DS 18.13 Tue 14:30 Poster A

Exciton diffusion length measurements on organic thin films for the application in photovoltaic cells — •Tobias Schuon, Tobias Roller, and Jens Pflaum — 3. Physikalisches Institut, Universität Stuttgart, D-70550 Stuttgart

The exciton diffusion length, L_D, has an important impact on the efficiency of photovoltaic devices. Therefore the detailed knowledge of the dependence of this quantity on the structural and chemical sample properties is crucial for PV cell optimization. In this work L_D has been measured by photoluminescence quenching on layers of various materials, viz. DIP (diindenoperylene), CuPc and PTCBI, and at different thicknesses. Alternatively, we estimated L_D via the spectral PV photocurrent on the basis of a suited exciton diffusion model[1]. To achieve a complete set of material and device parameters, comprehensive studies by X-ray diffraction, UV-Vis spectroscopy and AFM have been performed.

As a key result, DIP provides an exciton diffusion length in the order of 100 nm, thereby compensating for its rather weak absorption[2]. We related this high L_D to the fact, that DIP forms a structural phase of high crystallinity on weakly interacting substrates, with its long molecular axis preferentially oriented along the surface normal[3]. Furthermore, balanced electron and hole mobilities along this crystallographic direction support the application of DIP in PV devices[4].

[1] A.K.Ghosh, T.Feng, J.Appl.Phys. **49**, 5982 [2] D.Kurrle, J.Pflaum, Appl.Phys.Lett. (subm.) [3] A.C.Dürr, et al., Appl.Phys.Lett. **81**, 2276 [4] A.K.Tripathi, J.Pflaum, Appl.Phys.Lett. **89**, 82103

DS 18.14 Tue 14:30 Poster A

Nanocolloidal Scattering Particles Integrated in OLEDs — •Boris Riedel, Julian Hauss, Sebastian Gleiss, Uli Lemmer, and Martina Gerken — Lichttechnisches Institut, Universität Karlsruhe (TH)

Organic light emitting devices (OLEDs) combine cost-effective fabrication with large device areas. While OLEDs are starting to appear in commercial displays, they are not sufficiently bright yet for lighting applications. In current OLEDs only about 20% of the generated photons can exit the device. The rest is trapped as surface plasmon polaritons or as guided modes inside the organic layers or the substrate. We investigate the influence of nanocolloidal scattering particles on the extraction efficiency of OLEDs. These particles inhibit internal guided modes inside the OLED and thus increase the amount of extracted light. We use SiO2 and ZnO dispersed in water and ethyl alcohol respectively and bring them onto the Indium Tin Oxide-anode. This modified substrate is then further processed by evaporating small molecules or by spincoating polymers. Fabricated devices are characterized electrically and optically.

DS 18.15 Tue 14:30 Poster A

***in vivo* STM-observation of the growth of 3,4,9,10 perylene tetracarboxylic (PTCDA) crystals on Si(111)** 7×7 — •Thorsten Wagner[1], Rolf Möller[1], Masafumi Sakata[2], and Kingo Itaya[2] — [1]Universität Duisburg-Essen, Fachbereich Physik, Lotharstr. 1-21, 47057 Duisburg — [2]Tohoku University, Department of Applied Chemistry, Sendai, Japan

We will show scanning tunnelling microscopy (STM) results on the *in vivo* observation of the growth of organic nanocrystals. 3,4,9,10 perylene tetracarboxylic dianhydride (PTCDA) was thermally evaporated onto a clean Si(111) 7×7 surface held at room temperature. A sequence of images acquired over a period of 24h shows how the unordered structure with no visible molecular resolution evolves to individual crystals which can be well characterized. The size of the crystallites (roughly 10nm by 10nm) is consistent with former thermal desorption experiments (TDS) of PTCDA on Cu(111): The number of crystals increases with the coverage. This can be related to the higher the density of nucleation centres. Between preparation and first imaging had been 12h. In addition, the formation of the crystals took place during the STM obervation. Therefore we propose that the growth of the crystals is not only driven by diffusion. By operating the STM at mean current of 2pA and a bias voltage of +1.5V the tip adsorbat interaction was minimized. Anyway this small force could be enough to push and drag the molecules into the energetically preferred adsorption sites within the crystalline structures. Once the crystalline structures have been formed the images were stable and molecular resolution was possible.

DS 18.16 Tue 14:30 Poster A

Growth monitoring of CuPc on H-Si(100) and In/CuPc interface formation Studied by Raman Spectroscopy — Marius Toader, •Philipp Schäfer, Cameliu Himcinschi, and Dietrich R T Zahn — Chemnitz University of Technology, Semiconductor Physics, D-09107, Chemnitz, Germany

Copper phthalocyanine (CuPc) layers deposited under ultra high vacuum conditions using organic molecular beam deposition onto hydrogen passivated silicon H-Si(100) substrates were investigated using Raman spectroscopy. Different emission lines (from 488 nm to 676 nm) of Ar or Kr lasers were used for excitation in a backscattering geometry. *In situ* on-line growth monitoring was performed in order to determine influence of the thickness on the internal molecular vibrations. The Raman spectra, recorded in different polarization configurations, macro and micro configurations, *in situ* and *ex situ* respectively, were used to estimate the orientation of CuPc molecules in the layers. Novel devices based on organic semiconductors such as organic field effect transistors or organic light emitting diodes require metallic contacts. Therefore, the interface between metals and organic semiconductors require special attention. *In situ* Raman scattering was thus also employed to assess the In/CuPc interface formation.

DS 18.17 Tue 14:30 Poster A

Nanostructures to Enhance Light Extraction from OLEDs — •Julian Hauss, Sebastian Gleiss, Ulf Geyer, Boris Riedel, Uli Lemmer, and Martina Gerken — Lichttechnisches Institut, Universität Karlsruhe, D-76131 Karlsruhe, Germany

In current organic light emitting diodes (OLEDs) only a small fraction of the generated photons can be extracted as useful light (5-20%). Besides quenching and substrate modes, guided modes in the organic layers and surface plasmons at the metal-organic interface are the main loss channels. The outcoupling of substrate modes is widely studied and established in common devices whereas for the outcoupling of guided modes and plasmons a general remedy is still lacking. We study the angular and spectral dependence of the emitted light and the ability to tailor these properties by periodic nanostructures, which scatter guided modes and surface plasmons. The investigated structures are fabricated by interference lithography, which is a promising approach to large scale and cost effective production. The experimental results are compared to numerical simulations.

DS 18.18 Tue 14:30 Poster A

AFM Lithography on Polymer Brushes and Spin-Coated Polymer Films — •Michael Hirtz[1], Marion K. Brinks[2], Armido Studer[2], Harald Fuchs[1], and Lifeng Chi[1] — [1]Physikalisches Institut, Westfälische Wilhelms-Universität, Wilhelm-Klemm-Straße 10, 48149 Münster, Germany — [2]Organisch-Chemisches Institut, Westfälische Wilhelms-Universität, Corrensstraße 40, 48149 Münster, Germany

Polymer brushes offer an interesting route to tailor surface properties [1]. Additionally it is of great interest to generate structured polymer brushes [2,3,4]. Here we present our investigation on the properties of different polymer brushes (polystyrene (PS), polyacrylate (PA) and poly(n-isopropylacrylamide) (PNIPAM)) with a thickness of 5 to 50nm grafted onto siliconoxide used as substrates for AFM lithography. In comparison to spin-coated polymer films of similar thickness, polymer brushes exhibit enhanced mechanical properties in regard to pattern fidelity, stability and resolution. The resulting patterns can be used as masks and templates for further lithographic steps.

[1] Y. Tsujii, K. Ohno, S. Yamamoto, A. Goto, T. Fukuda; Adv. Polym. Sci. (2006) 197: 1-45. [2] K.D. Dronavajjala, R. Rajagopalan, S. Uppili, A. Sen, D.L. Allara, H.C. Foley; J. Am. Chem. Soc. (2006) 128: 13040-13041. [3] Y. Tsujii, M. Ejaz, S. Yamamoto, T. Fukuda, K. Shigeto, K. Mibu, T. Shinjo; Polymer (2002) 43: 3837-3841. [4] M.K. Brinks, M. Hirtz, L.F. Chi, H. Fuchs, A. Studer; Angew. Chem. Int. Ed. (2007) 46: 5231-5233.

DS 18.19 Tue 14:30 Poster A

Temperature dependent measurements on perylene thin-film based OTFTs — •Christian Effertz, Moritz Schaefer, Maryam Beigmohamadi, Azadeh Farazadi, Phenwisa Niyamakom, Philip Schulz, and Matthias Wuttig — Institute of Physics (IA), RWTH Aachen University, 52056 Aachen, Germany

Organic Thin-Film Transistors (OTFTs) are promising candidates for electronic applications, e.g. as an active matrix for flexible displays. Some organic materials, such as perylene, show a high field-effect mobility, comparable to hydrogenated amorphous silicon (a-Si:H). In order to describe the mechanism of charge transport, competing models, like the grain boundary model, the small polaron model and the multiple trapping and release model have been developed in the past. However, for a wide range of organic semiconductors it is not yet understood what model has to be applied. In order to gain a deeper insight into the transport meachnisms of organic materials we present temperature dependent measurements of the electronic transport in perylene-based OTFTs. The temperature range between 213K and 418K has been investigated. The TFTs were produced employing OTS and 2-propanol modified SiO_2 dielectric layers, on top of highly doped silicon substrates, which were used as the gate contact. Thermally evaporated gold pads acted as the contacts for the source and drain of the devices. Besides electronic measurements, additional characterization techniques, including Atomic Force Microscopy (AFM) for the surface morphology and X-Ray Diffractometry (XRD) for structural analysis of the organic layer have been employed in this investigation.

DS 18.20 Tue 14:30 Poster A

LT-STM study of indivdual CuPc molecules on Cu(111) — Hatice Karacuban, •Johannes Schaffert, Sascha Koch, Thorsten Wagner, and Rolf Möller — Universität Duisburg-Essen, Fachbereich Physik, Lotharstr. 1-20, 47057 Duisburg

The interface between organic semiconductors and metals plays a key role for the electronic properties and thus for their application in devices. We present a low temperature scanning tunneling microscopy and spectroscopy study of copper phthalocyanine on Cu(111). A submonolayer of CuPc was evaporated onto a clean Cu(111) single crystal at room temperature under ultra high vacuum (UHV) conditions. Previous measurements show that at room temprature single CuPc molecules are mobile on the Cu(111) surface and can not be imaged by means of STM. The presented STM measurements have been carried in UHV at temperatures below 10K. We observe CuPc adsorbed in two different geometries, as well as the equivalent sites, rotated by multiples of 60°. One of the adsorption sites leads to an apparent reduction of the molecules four-fold symmetry in the STM image. Two opposite of four benzopyrrol rings appear brighter. First spectroscopic results show, that the brighter parts also differ electronically. Furthermore, the molecules adsorbed with reduced symmetry tend to align forming chains of molecules on the Cu(111)surface.

DS 18.21 Tue 14:30 Poster A

Ellipsometry Investigation of Pentacene Thin Films — •Marion Friedrich, Daniel Lehmann, Falko Seidel, and Dietrich R. T. Zahn — TU Chemnitz, Institut für Physik, 09107 Chemnitz, Germany

Thin pentacene layers with thicknesses ranging between 20 and 150 nm were prepared by organic molecular beam deposition on native oxide covered silicon substrates. Variable angle spectroscopic ellipsometry was applied aiming at the determination of thicknesses and dielectric function of pentacene thin films. Starting with the assumption that the optical properties are the same, the optical constants of several films with different thickness were coupled and fitted together with the film thicknesses in a multi-sample analysis procedure. For thickness determination different models are employed and discussed regarding their deviation from the measurement results. Best agreement between simulation and experiment was found for a model implying uniaxial films. As a result of further detailed data evaluation in the absorbing spectral range a difference in the dielectric functions for thin and thick layers was determined.

DS 18.22 Tue 14:30 Poster A

Spectroscopic studies of metal oxide sensitisation by self-assembling light harvesting molecules and photovoltaic applications — •Clare Dyer-Smith[1], Jenny Nelson[1], Saif A Haque[2], Peter Marek[3], and T Silviu Balaban[3] — [1]Dept of Physics, Imperial College, London SW7 2AZ, U.K — [2]Dept of Chemistry, Imperial College, London SW7 2AZ, U.K — [3]Karlsruhe Institute of Technology, Institute for Nanotechnology, Postfach 3640, D-76021 Karlsruhe

Molecular photovoltaic devices may provide a low-cost alternative to crystalline silicon solar cells with the long-term potential to displace conventional fossil fuels. Naturally occurring within green photosynthetic bacteria are metal porphyrins which self assemble to form a light harvesting antenna architecture enabling exciton transport over longer ranges. This is promising for application in organic solar cells where charge separation requires exciton diffusion to an interfacial site. Self assembly is thought to lead to improved charge transport properties and therefore improved photocurrent generation efficiency. We report studies of functionalised porphyrins acting as the donor component in molecular photovoltaic devices. We study the influence of film morphology, influenced by the porphyrin side groups, on exciton diffusion, charge separation yield and charge transport in porphyrin films on semiconducting metal oxide surfaces. Charge separation and transport properties are measured using transient optical spectroscopy and time of flight techniques and are correlated to film morphology. The structure and energetics of the donor-acceptor interface are key to maximising the potential of such systems for photovoltaic applications.

DS 18.23 Tue 14:30 Poster A

Investigation of thermally activated charge carrier transport in thin perylene layers — •Moritz Schaefer, Christian Effertz, Maryam Beigmohamadi, Phenwisa Niyamakom, Azadeh Farahzadi, Philip Schulz, and Matthias Wuttig — Institute of Physics (IA), RWTH Aachen University, 52056 Aachen, Germany

The production of organic thin-film transistors (OTFTs) is a low cost process. Therefore, they are promising for large area TFT arrays as needed in low cost electronic paper, RFID tags, etc. [1]. Recently reported characteristics of OTFTs in terms of mobility and Ion/Ioff-ratio are similar to those of the currently used hydrogenated amorphous silicon (a-Si:H) TFTs [1]. It is now possible to produce OTFTs with a comparable high performance, but the transport phenomena in the organic layer are still not completely understood.

We present the electronic characteristics of perylene based OTFTs. Transfer and output characteristics were measured in order to determine the mobility μ(T) and the threshold voltage VT(T). For this purpose, a stage was designed that can be cooled to -50°C and heat to +100°C. The active layer of the transistors was produced by vacuum thermal evaporation (VTE) via a temperature controlled substrate holder with a temperature range from -40°C to +35°C. The organic film thickness was varied between 25 nm and 500 nm. Atomic Force Microscopy (AFM) and x-ray diffraction (XRD) have been used in order to determine the crystallinity and morphology of the organic layer.

[1] D. S. Park, et. al., J. Vac. Sci. Technol. B 23(3) (2005)

DS 18.24 Tue 14:30 Poster A

Mobile Ionic Impurities in Organic Thin Film Dielectrics for Electronic Application — •Reinhard Schwödiauer[1], Martin Egginger[2], Mihai Irimia-Vladu[1], Andreas Tanda[4], Irene Frischauf[3], Siegfried Bauer[1], and Serda Sariciftci[2] — [1]Soft Matter Physics, Johannes Kepler University, Altenbergerstrasse 69, 4040 Linz, Austria — [2]Linz Institute for Organic Soloar Cells, Johannes Kepler University, Altenbergerstrasse 69, 4040 Linz, Austria — [3]Institute for Biophysics, Johannes Kepler University, Altenbergerstrasse 69, 4040 Linz, Austria — [4]Plastic Electronics GmbH, Rappetsederweg 28,4040 Linz, Austria

In the field of organic electronics organic thin film dielectrics can have a strong influence on the device performance. We present a comprehensive and comparative study of mobile ionic impurities for BCB and poly(vinyl alcohol) with traces of sodium acetate at different concentrations, ranging from below 0.004 mass% up to < 0.5 mass%. The two polymers are investigated both in a metal-insulator-metal (MIM) and a metal-insulator-(C60) semiconductor (MIS) configuration by broadband dielectric spectroscopy in the frequency-(50 *H < f < 10 kHz), dc bias voltage (-25 V < Ubias < +25 V) and temperature (20°C < T < 120°C) domain. In addition we also present measurements on OFETs of the same material combination at different temperatures between 3°C and 60°C.

The consistent results show conclusive evidence for the impact of mobile ions in organic dielectrics for the stability and reliability of organic field effect transistors.

DS 18.25 Tue 14:30 Poster A

Design and Performance of an Ion Beam Vacuum Deposition Apparatus Based on Electrospray Ionization — •Stephan

Rauschenbach, Nicha Thontasen, Ralf Vogelgesang, Giovanni Costantini, Nicola Malinowski, and Klaus Kern — Max-Planck-Institute for Solid State Research, Stuttgart, Germany

An electrospray (ES) ion beam deposition apparatus has been developed for the high- and ultrahigh vacuum (UHV) deposition of non-volatile molecules and nanoparticles. The source employees electrospray ionization to create gas phase ions, RF-quadrupoles and electrostatic ion optics for the formation and the guiding of the ion beam, differential pumping to overcome the vacuum gap to UHV and a time-of-flight mass spectrometer for in-situ characterization of the ion beam before deposition.

The ion beam is deposited on sample holders in high- and ultrahigh vacuum designed for ex-situ or in-situ analysis respectively. The parameters of the deposition, ion beam current and kinetic energy are measured and controlled before deposition, which together with the mass analysis gives complete control over the experiment. The apparatus is connected to an STM/AFM for in-situ analysis.

Time-of-flight mass spectrometry and ion beam deposition of small molecules, large biomolecules and nanoparticles is illustrated in some examples. Fluorescent molecules are used as soft landing probes, single and double layer islands of amphophilic molecules are grown and large nanoparticles can be deposited.

DS 18.26 Tue 14:30 Poster A

Structural, Morphological, and Optical Properties of Tetraphenylporphyrin Films on Silicon Substrates — •Simona Pop[1], Tobat Saragi[2], Sylvia Wenmackers[3], Josef Salbeck[2], Patrick Wagner[3], and Norbert Esser[1] — [1]ISAS-Institute for Analytical Sciences, Department Berlin, Albert-Einstein Str. 9, D-12489, Berlin, Germany — [2]Macromolecular Chemistry and Molecular Materials (mmCmm), Department of Science and Center for Interdisciplinary Nanostructure Science and Technology (CINSaT), University of Kassel, Heinrich-Plett Strasse 40, D-34109 Kassel, Germany — [3]Hasselt University, Institute for Materials Research, Wetenschapspark 1, 3590 Diepenbeek, Belgium

Thin films of free base-meso-tetraphenylporphyrin (H2TPP) grown by organic molecular beam deposition on silicon substrates are characterized by means of spectroscopic ellipsometry, scanning electron microscopy, and atomic force microscopy techniques. The anisotropic dielectric function of H2TPP films is determined in the photon energy range from 0.73 to 5 eV. The imaginary part of the dielectric function exhibits the typical Q and Soret bands. The Q band (pi-pi* transition) displays the typical vibrational structure consisting of the following subbands Qx(0,0) at 1.90 eV, Qx(1,0) at 2.08 eV, Qy(0,0) at 2.2 eV, and Qy(1,0) at 2.38 eV. It is observed only for the in-plane component of the dielectric function meaning that most of the H2TPP molecules adopt a planar orientation with respect to the substrate surface. The thickness dependence of the dielectric function of the H2TPP films is additionally discussed.

DS 18.27 Tue 14:30 Poster A

XPS and ARPES studies of azobenzene derivatives on layered materials — •Jaroslaw Iwicki, Tilo Peter, Kai Rossnagel, and Lutz Kipp — Institut für Experimentelle und Angewandte Physik, Universität Kiel, D-24098 Kiel, Germany

Derivatives of azobenzene with different dipole moments were deposited onto layered materials. The preparation process allows the deposition of low sublimation point molecules on a crystal surface under UHV conditions with a marginal contamination of residual gas atoms. The tube with the molecules is vacuum pumped, cooled in a nitrogen bath, heat sealed and placed in the UHV preparation chamber. The deposition process starts when the seal is broken. XPS and ARPES measurements have been carried out at the BW3 beamline at HASYLAB. XPS measurements confirm the adsorption of the azobenzene derivatives on the substrate and ARPES measurements disclose the valence electronic structure of the molecules on the crystal surface.

DS 18.28 Tue 14:30 Poster A

Continuous Wavelength Tuning in a Wedge-Shaped Organic Microcavity Laser — •Bernd Schütte, Hannes Gothe, Susanne I. Hintschich, Markas Sudzius, Hartmut Fröb, Vadim G. Lyssenko, and Karl Leo — Institut für angewandte Photophysik, TU Dresden, George-Bähr-Str. 1, 01069 Dresden

Due to their broad gain spectra, lasers consisting of organic materials offer the prospect of wavelength tuning over a wide spectral range. We demonstrate a continuously tunable organic microcavity laser. Two distributed Bragg reflectors (DBRs) serve as mirrors, which are grown by reactive electron-beam evaporation. Each DBR consists of 10 alternating pairs of $\lambda/4$ layers. A guest-host composite of Alq_3 and DCM is used as the gain medium. This active layer is conveniently fabricated by thermal co-evaporation, which utilizes a rotating shadow mask in order to produce a wedge shape. Wavelength tuning is achieved by ac variation of the pump beam position on the microcavity, thus changing the resonance condition in the active layer. Its wedge-shaped profile allows to continuously select any wavelength between 595 nm and 650 nm. Thus, we scan the gain spectrum of the active medium, enabling us to optimise the laser threshold. Further scope to expand this range is provided by the high chemical stability of the organic material, which allows to pump at intensities of up to three orders of magnitude beyond the lasing threshold.

DS 18.29 Tue 14:30 Poster A

Influence of inhomogeneous broadening on the input-output characteristics of an organic microcavity — •Susanne I. Hintschich, Hannes Gothe, Markas Sudzius, Hartmut Fröb, Vadim G. Lyssenko, and Karl Leo — Institut für angewandte Photophysik, TU Dresden, George-Bähr-Str. 1, 01069 Dresden

We investigate the input-output characteristics of a continuously tunable organic vertical cavity surface emitting laser (OVCSEL). The microcavity consists of two distributed Bragg reflectors, which enclose an active layer of the guest:host system Alq_3:DCM. The wedge-shaped geometry of this layer enables us to scan the input-output curves across the entire gain spectrum of DCM, using a single sample. Due to the high chemical stability of the material, we can reversibly monitor the behaviour over more than 2 orders of magnitude beyond the lasing threshold at the maximum of the gain spectrum. All input-output curves deviate strongly from the standard model for homogeneously broadened emitters, which uses a single spontaneous emission factor, beta. Therefore, we take into account the inhomogeneous broadening of the organic material by introducing a distribution of beta factors. Depending on the type, width and spectral position of this distribution with respect to the cavity mode, the shape of the model curve is altered. Eventually, a Gaussian distribution with suitable parameters is used to represent the inhomogeneously broadened gain spectrum of DCM. Thus, we qualitatively model the input-output behaviour of an organic microcavity laser and demonstrate the impact of inhomogeneous broadening.

DS 18.30 Tue 14:30 Poster A

Infrared spectroscopical studies of the evaporation, condensation and annealing process of SiO_2 — •Michael Möller, Markus Klevenz, and Annemarie Pucci — Kirchhoff-Institut für Physik, Universität Heidelberg, Im Neuenheimer Feld 227, 69120 Heidelberg

For several reasons silicon oxides are materials of persistently big interest, from astronomy to microelectronics. We studied the evaporation, condensation and annealing process of SiO_2 under ultra-high vacuum (UHV) conditions with *in-situ* infrared (IR) spectroscopy. All measurements were performed in an UHV chamber with base pressure below 5×10^{-10} mbar. First the equilibrium vapour pressure of quartz (SiO_2) was determined by measuring the molecular flow from a tantalum Knudsen cell onto a quartz microbalance. Afterwards the evaporated material was deposited on different substrates with appropriate IR and thermal properties (Si, Ge, Ta). The condensation process was observed with IR transmittance (on Si, Ge) and IR reflectance spectroscopy (on Ta). The observed spectra revealed the optical properties of SiO_x with the strongest Si-O stretching vibration bands at 990 and 1125 cm^{-1}. After annealing gradually to temperatures of up to 800°C a peak shift to 1070 and 1190 cm^{-1} was observed, respectively, before complete desorption at about 900°C occurred. The peak shifts can be explained by decomposition of the initial SiO_x into Si and SiO_2.

DS 18.31 Tue 14:30 Poster A

Evaporation, condensation and annealing of forsterite studied by infrared spectroscopy — •Markus Klevenz[1], Michael Möller[1], Mario Trieloff[2], Dominique Lattard[2], and Annemarie Pucci[1] — [1]Kirchhoff-Institut für Physik der Universität Heidelberg, Deutschland — [2]Mineralogisches Institut der Universität Heidelberg, Deutschland

Forsterite (Mg_2SiO_4) is a silicate that plays a crucial role in the formation of planets and, therefore, it is of special interest in astronomy and mineralogy. Its optical phonons determine the infrared (IR) absorption and emission of protoplanetary disks. For a better under-

standing of the formation of the silicate compounds and the observed IR spectra, the physical and chemical properties of forsterite and later on those of other relevant silicates will be investigated in laboratory studies under well-defined similar conditions (UHV). First, the vapour pressure curves and the composition of the gas phase will be determined. This will be realized by evaporation from a Knudsen cell with defined temperatures and measuring the molecular flow onto a quartz microbalance and the composition by mass spectroscopy. Afterwards the minerals will be deposited on a substrate and characterized *in situ* by IR spectroscopy to gather information about the condensation process. Subsequently the deposited films will be annealed up to 1200 K to observe the phase transition from amorphous to crystalline *in situ* by IR spectroscopy for determining characteristic temperatures and times of the crystallization process.

DS 18.32 Tue 14:30 Poster A

In-situ monitoring of electrochemically prepared organic films — •Karsten Hinrichs[1], Simona Silaghi[1], Matthias Intelmann[2], Katy Roodenko[1], Norbert Esser[2], and Jörg Rappich[1] — [1]ISAS - Institute for Analytical Sciences, Department Berlin, Albert-Einstein-Str. 9, 12489 Berlin, Germany — [2]Hahn-Meitner-Institut Berlin GmbH, Abt. Silizium-Photovoltaik, Kekuléstr. 5, 12489 Berlin, Germany

In-situ investigations of Si surfaces during electrochemical modification can elucidate reaction schemes and process steps. Such studies provide information about intermediate surface species during processing and species post-formed after the treatment in solution. Grafting of organic molecules is a widely used process to functionalize the silicon surface with respect to nanopatterning, passivation or change in electronic properties. In the presented work infrared spectroscopic ellipsometry (IRSE) and reflectance anisotropy spectroscopy were applied for in-situ monitoring of the electrochemical growth of thin organic films at the silicon-liquid interface. In particular the spectra taken during the growth of a few nm thick polypyrrole and nitrobenzene films will be discussed.

DS 18.33 Tue 14:30 Poster A

Molecular orientation in Au-molecular layer-GaAs diodes studied by IR ellipsometry — •Dana Maria Rosu[1], Aaron Trionfi[3], Julia Hsu[3], Karen Kavanagh[4], Ullrich Schade[2], Norbert Esser[1], and Karsten Hinrichs[1] — [1]ISAS - Institute for Analytical Sciences, Department Berlin, Albert-Einstein-Str. 9, 12589 Berlin, Germany — [2]Berliner Elektronenspeicherring-Gesellschaft für Synchrotronstrahlung mbH, Albert-Einstein-Str. 15, 12589 Berlin, Germany — [3]Sandia National Laboratories, Albuquerque, New Mexico 87185- 1120 — [4]Kavanagh Lab, Dept. of Physics, Simon Fraser University, 8888 University Dr., Burnaby, BC, V5A 1S6, Canada

Synchrotron mapping IR ellipsometer at BESSY[1] was used for investigation of molecular orientation and lateral homogeneity in different organic-GaAs hybrid diodes with a lateral resolution below 1 mm2. Organic films on GaAs and Au are compared, the organic layer being either octanedithiol (C8DT), or hexadecanethiol (C16MT). Analysis of the CH2 stretching vibrations provides informations on the structure of the main backbone, while the CH3 stretching bands is giving informations about the structure and orientation of the end group of the molecules. The bands for C16MT on GaAs show a different orientation in comparison with C8DT. Evaluation of measured spectra with optical models enables spectra interpretation.

[1] M. Gensch, N. Esser, E. H. Korte, U. Schade, K. Hinrichs, Infrared Physics and Technology 49 (1-2) (2006) 39-44

DS 18.34 Tue 14:30 Poster A

Infrared Synchrotron Mapping Ellipsometry of biomolecular thin films — •Dana Maria Rosu[1], Ullrich Schade[2], Norbert Esser[1], and Karsten Hinrichs[1] — [1]ISAS- Institute for Analytical Sciences, Department Interface Spectroscopy, Albert-Einstein-Str. 9, 12489 Berlin, Germany — [2]BESSY GmbH, Albert-Einstein-Str. 15, 12489 Berlin, Germany

The IR synchrotron ellipsometer at BESSY II, for the mid infrared range, enables investigation of samples with monolayer sensitivity and a lateral resolution below 1 mm2. Being equipped with a mapping table [1], the set-up allows the investigation of heterogeneous organic thin films. In cooperation with Sentech Instruments the IR synchrotron mapping ellipsometer was upgraded with a rotating retarder. In the recent years IR ellipsometry has been applied for structural analysis of thin organic films [2]. Results from mapping ellipsometry of biosensors [3] and molecular monolayers, with thicknesses between 2 nm and 100 nm, will be presented. Evaluation of measured spectra with optical models gives informations about thickness, homogeneity and orientation of the molecules on the substrates.

[1] M. Gensch, N. Esser, E. H. Korte, U. Schade, K. Hinrichs, Infrared Phys. and Technol. 49(1-2)(2006) 39-44

[2] K. Hinrichs, M. Gensch, N. Esser, Appl. Spectrosc. 59 (2005) 272A-282A

[3] K. Hinrichs, M. Gensch, N. Esser, U. Schade, J. Rappich, S. Kröning, M. Portwich, R. Volkmer, Anal. and Bioanal. Chem. 387(5)(2007) 1823-1829

DS 18.35 Tue 14:30 Poster A

Online monitoring of the surface properties of mixed polymer brushes via in-situ infrared ellipsometry — •Dennis Aulich[1], Igor Luzinov[2], Olha Hoy[2], Leonid Ionov[3], Sergiy Minko[4], Klaus-Jochen Eichhorn[3], Manfred Stamm[3], Norbert Esser[1], Ulrich Schade[5], and Karsten Hinrichs[1] — [1]ISAS, Department Berlin, Albert-Einstein-Str. 9, 12489 Berlin — [2]Clemson University, Clemson, SC 29634-0971, USA — [3]IPF Dresden, Hohe Str. 6, 01069 Dresden — [4]Clarkson University, Potsdam, New York 13699, USA — [5]BESSY II, Albert-Einstein-Str. 15, 12489 Berlin

As a new type of functional surfaces, mixed polymer brushes offer a wide range of applications due to the possibility of changing the surface properties by external stimuli such as pH, solvent, light or electric field [1, 2]. Two different mixed polymer brushes were prepared using two subsequent "grafting to"procedures (a mixed P2VP-PAA and a mixed PEG-PAA/PS brush, each with 50/50 composition). The composition of the film was analyzed quantitatively by VIS-IR-ellipsometry. The in-situ-characterization was done by polarization dependent infrared (IR) ellipsometry in single reflection geometry both in the laboratory and in the synchrotron IR beamline at BESSY II. Exposure of the samples to different solutions at varying pH led to structural and chemical changes. Repeating cycles of systematic change of pH led to strong, reversible switching of the brush which was analyzed online via the component specific vibrational bands of the polymers.

References: [1] S. Minko et al., *Macromol. Rapid Commun.* **22**(3): 206, 2001; [2] L. Ionov et al., *Langmuir* **21**(19): 8711, 2005

DS 18.36 Tue 14:30 Poster A

Study of perylene films by Fourier transform infrared spectroscopy — •Li Ding, Kostiantyn V. Shportko, Philip Schulz, Azadeh Farahzadi, and Matthias Wuttig — Institute of physics (IA), RWTH Aachen University, 52056, Aachen, Germany

Organic semiconductors has attracted considerable attention recent years due to their potential application in electronic devices. Fourier transform infrared spectroscopy (FTIR), as a useful tool to study vibrational properties of molecules, contains information on the molecular orientation in films [1]. Since the molecular stacking has a significant impact on the electronic and optical properties of films, it is of great interest to understand the molecular orientation in thin films [2].

Thermally evaporated perylene films are grown on a silver layer deposited on glass substrates. Infrared reflectance spectra of perylene films on Ag/glass have been measured with the incident angle from 20° to 70°. The change of absorption intensities at different incident angles indicates that the average orientation of perylene molecules on Ag/glass tends to be perpendicular to the substrate surface. XRD pattern shows that thick perylene films are highly crystalline. We have compared the absorption frequencies and intensities of perylene film with those of isolated molecules. Some new frequencies are seen in the spectrum of crystalline perylene film, which are attributed to the dimer structure in the crystalline phase.

[1] D. L. Allara, J. D. Swalen, J. Phys. Chem. 86, 2700 (1982).

[2] K. Akers, R. Aroca, A. Hor, R.O. Loutfy, J. Phys. Chem. 91, 2954 (1987).

DS 18.37 Tue 14:30 Poster A

Tip-Enhanced Optical Microscopy of Single-Walled Carbon Nanotubes — •Carsten Georgi[1], Huihong Qian[1], Neil Anderson[2], Lukas Novotny[2], and Achim Hartschuh[1] — [1]Department Chemie und Biochemie & CeNS, Ludwig-Maximilians-Universität München, Germany — [2]University of Rochester, The Institute of Optics, Rochester, New York 14627, USA

Optical Microscopy with nanoscale spatial resolution is an essential technique for the detection and characterization of individual nanoobjects and nanostructured materials. We use the field enhancement in the proximity of a laser-illuminated sharp metal tip to locally excite and probe the optical response of nanoscale systems. In particular, we

image the vibrational and electronic properties of single-walled carbon nanotubes with a spatial resolution of down to 10nm, limited only by the tip diameter [1,2]. Local perturbations along an individual nanotube, as well as energetic coupling between different nanotubes can thereby be directly observed, revealing the interaction of phonons and excitons with the nanotube structure and its environment.

[1] A. Hartschuh et al., Nano Lett. 5, 2310 (2005)
[2] N. Anderson et al., Nano Lett. 7, 577 (2007)

DS 18.38 Tue 14:30 Poster A

Vibrational Study of Free-Base Tetraphenylporphyrin Films — •Simona Dorina Pop, Dana Maria Rosu, Karsten Hinrichs, and Norbert Esser — ISAS-Institute for Analytical Sciences, Department Berlin, Albert-Einstein Str. 9, D-12489, Berlin, Germany

The vibrational structure of the vacuum deposited free-base mesotetraphenylporphyrin (H_2TPP) films on silicon substrates is investigated by infrared spectroscopic ellipsometry. The dielectric function of the H_2TPP films is determined in the mid-infrared energy range. The H_2TPP films exhibit a uniaxial structure in agreement with the results obtained by spectroscopic ellipsometry performed in the visible energy range. The orientation of the H_2TPP molecules on silicon substrates as well as the thickness dependence of the IR dielectric function are analyzed. The assignment of the observed vibrational bands is performed with the help of density functional theory method.

DS 18.39 Tue 14:30 Poster A

Application of Raman Spectroscopic Techniques in the Characterization of Nanostructured Semiconductors and Semiconductor Microstructures — •Dimitra Papadimitriou — National Technical University of Athens, Faculty of Applied Sciences, Department of Physics, GR-15780 Athens, Greece

Applications of Raman spectroscopic techniques in basic and applied research studies are reviewed. Emphasis is given to the characterization of structural phases, phase-transformation, and nanometric scale effects in nanostructured semiconductors by Raman and the validation of strain-stress effects in semiconductor microstructures by micro-Raman Spectroscopy. In particular: a) applications of combined Raman scattering and photoluminescence emission techniques in the determination of the pressure dependence of the energy band-gap and the transformation pressure of nanocrystalline (porous) silicon under high hydrostatic pressure are presented [1], b) applications of the Raman selection rules in the structural characterization of light emitting silicon quantum wires are discussed [2], and c) the relevance of micro-Raman techniques for the characterization of elastic strain in porous silicon microstructures is demonstrated [3].

References: [1] D. Papadimitriou, Y.S. Raptis and A.G. Nassiopoulou, Phys. Rev. B 58(21), 14089, (1998). [2] D. Papadimitriou and A.G. Nassiopoulou, J. Appl. Phys. 84(2), 1059 (1998). [3] D. Papadimitriou, C. Tsamis, A. Nassiopoulou, Sensors and Actuators B: Chemical 103(1-2), 356 (2004).

DS 19: Organic Interfaces (SYSA 6)

Time: Wednesday 14:30–17:30 Location: H 2013

Invited Talk DS 19.1 Wed 14:30 H 2013

Organometallic Nanojunctions Probed by Different Chemistries: Thermo-, Photo, and Mechanochemistry — •I. Stich[1,2], M. Konopka[1], R. Turansky[1], J. Reichert[3], N. L. Doltsinis[4], H. Fuchs[3], and D. Marx[4] — [1]Slovak Tech. Univ. (FEI STU), Slovakia — [2]Inst. of Phys., Slovak Acad. of Sci., Slovakia — [3]Uni. Muenster, Germany — [4]Ruhr-Uni. Bochum, Germany

Different methods of activation of chemical reactions are compared for organometallic nanojuctions. The study is based on density functional theory simulations. First we provide a comparison of thermal activation with mechanical activation, or mechanochemistry. Study of thiolate/copper junctions and interfaces provides evidence for vastly different reaction pathways and products. The differences are understood in terms of mechanical manipulation of coordination numbers and system fluctuations in the process of mechanical activation. Next we compare photo- and mechanochemistry. Azobenzene is an optically switchable molecule. Laser light is normally used to achieve molecular switching between the cis and trans isomers. We study azobenzene optomechanical switch which combines photo excitation with external pulling force to manipulate optical switching properties of the azobenzene molecule anchored to gold tips by thiolate bonds. We focus on the separation between ground (S0) and first excited (S1) singlet states. We observe a pronounced dependence of the S0-S1 separation on the applied strain. Furthermore we find that ground-state mechanochemistry alone can be used to achieve switching. For instance, mechanochemistry with modest applied forces leads to cis -> trans reisomerization.

DS 19.2 Wed 15:00 H 2013

Self-Assembled Monolayers of Azo-based molecular switches — Andrei Shaporenko[1], Mark Elbing[2], Alfred Blaszczyk[2], Violetta Ferri[3], Christian Grave[3], Giuseppina Pace[4], Carsten von Hänsich[2], Marcel Mayor[2,5], Paolo Samorì[4], Maria Anita Rampi[3], and •Michael Zharnikov[1] — [1]Angewandte Physikalische Chemie, Universität Heidelberg, D-69120 Heidelberg, Germany — [2]Forschungszentrum Karlsruhe GmbH, Institute for Nanotechnology, D-76021 Karlsruhe, Germany — [3]Dipartimento di Chimica, Università di Ferrara, I-44100 Ferrara, Italy — [4]Institut de Science et d'Ingénierie Supramoléculaires / CNRS UMR 7006 -Université Louis Pasteur, F-67000 Strasbourg, France — [5]Department of Chemistry, University of Basel, CH-4056 Basel, Switzerland

Two conjugated rod-like aromatic azo-compounds differing by molecular conformation (planar vs. twisted) and required free volume (upon assembly) have been synthesized. While the first compound forms tightly packed self-assembled monolayers (SAMs) on coinage metal substrates with a high degree of ordering, the second one packs more loosely giving less ordered films. However, independent of the package density, both compounds show very high yields of photoisomerization in SAMs, which are close to 100%. This result questions the common believe that isomerization in SAMs of azo-compounds can only be achieved efficiently, when enough free volume is available in the monolayer. We conclude that azo units incorporated in rigid molecular rods can be of potential interest in molecular electronic devices for applications such as switchable devices and high density data storage.

DS 19.3 Wed 15:15 H 2013

Structural and optical properties of self-organized surface structures on rubrene single crystals — •Rainer Stöhr[1], Gareth Beirne[2], Peter Michler[2], Jörg Wrachtrup[1], and Jens Pflaum[1] — [1]3. Physikalisches Institut, Univ. Stuttgart,Germany — [2]IHFG, Univ. Stuttgart, Germany

On the surface of rubrene single crystals high hole mobilities up to 15 cm^2/Vs have been observed making this material interesting for organic device applications. However, the optical properties of rubrene single crystals are yet barely analysed.

We present first structural and optical studies on sublimation grown rubrene single crystals with self-organized pyramidal microstructures on the (001) surfaces. From OMBD growth at various conditions we conclude on the stabilization mechanisms of these crystallographically aligned structures.

Measuring the time- and locally-resolved micro-photoluminescence at various positions on the structured rubrene (001) surface, four peaks could be identified in the wavelength range between 500nm and 900nm. The generated microstructures on the crystal surface enhanced the peak intensities by up to an order of magnitude. A clear dependence between structure size and enhancement could be shown. The results are carefully discussed by assigning these peaks to various exciton species with respect to studies currently reported in literature [1].

The DFG (projects WR28/5 and FOR 730) is acknowledged for financial support.

[1] H. Najafov *et al.*, PRL **96**, 056604 (2006)

DS 19.4 Wed 15:30 H 2013

Monitoring the crystallization process of nano-confined organic molecules — •Silvia Milita[1], Chiara Dionigi[2], Francesco Borgatti[2], William Porzio[3], Adina Lazar[2], Roberto Felici[4], Didier Wermeille[4], and Fabio Biscarini[2] — [1]CNR -IMM, Via Gobetti 101, I-40129 Bologna, Italy — [2]CNR -ISMN, Via Gobetti 101, I-40129

Bologna, Italy — [3]CNR-ISMAC Via E. Bassini 15, I-20133 Milano, Italy — [4]ESRF-bp 220, F-38043 Grenoble Cedex 9, France

In the recent years crystallisation behaviour upon nano-confinement has drawn extensive attention thanks to its potential application in nanotecnhologies. Production of new functional materials requires the understanding of crystallization phenomena in complex systems as emulsions, vescicles, micelles, air-water interfaces, ordered substrates. We will report on the dynamical X-ray diffraction investigation of the structure of organic semicondutor molecules in confined systems which are highly attractive for their application in electronic-optoelectronic devices as Organic Field Effect Transistor (OFET).

DS 19.5 Wed 15:45 H 2013

A molecular gas in two dimensions: Substrate-mediated repulsive interaction in an organic sub-monolayer film — •Christian Kumpf[1], Achim Schöll[1], Christoph Stadler[1], Ingo Kröger[1], and Eberhard Umbach[1,2] — [1]Universität Würzburg, Experimentelle Physik II, 97074 Würzburg — [2]Forschungszentrum Karlsruhe, 76133 Karlsruhe

The formation of the first molecular layer on a solid surface plays an important role for the growth behaviour of organic thin films. The first layer acts as a nucleus for further growth. It hence affects the structural properties of the entire film and consequently the electronic and optical properties. The development of the first layer depends strongly on the substrate bonding and the intermolecular interaction. Usually the latter is attractive due to van-der-Waals forces between the organic molecules thus resulting in island formation.

Here we report on an organic adsorbate system exhibiting repulsive intermolecular interaction mediated by the substrate. With increasing coverage Metal-Phthalocyanine (MePc) molecules continuously rearrange on a Ag(111) surface and – at all coverages – fill the entire surface homogenously. This is in contrast to discrete, well defined phase transitions which usually occur for such systems. Such unusual behaviour was found for Sn-, Cu- and TiOPc molecules. We report experimental results from spot-profile analysis-low energy electron diffraction, x-ray standing waves and photoelectron spectroscopy, and discuss an electronic donation/back-donation process as the fundamental origin of the intermolecular repulsion.

DS 19.6 Wed 16:00 H 2013

Influence of Intermolecular Bonding on Interface Barrier Formation of $ZnPcCl_8$ on Ag111 Observed by Kelvin Probe Force Microscopy — •Peter Milde[1], Christian Loppacher[2], Ulrich Zerweck[1], Mireille Mossoyan[2], and Lukas M. Eng[1] — [1]Institut für Angewandte Photophysik, Technische Universität Dresden — [2]Laboratoire de Matériaux et Microélectronique de Provence, Universités Paul Cézanne, Marseille

Phthalocyanines are a common class of organic dyes for applications in optoelectronic devices. Compared to the standard phthalocyanine, halogenated phthalocyanine shows a different and more complex bonding behavior. Within the first monolayer of $ZnPcCl_8$ on Ag111 distinct structural phases where observed, which can be attributed to the formation of 8, 4 and no intermolecular hydrogen-halogenide bonds[1].

FM-KPFM measurements reveal, that the bonding behavior does not only affect the structural ordering but also the electronic properties of the molecule and thus the interface barrier formation. Furthermore, a reversed sign of the contact potential change is found between ordered and disordered molecular layers.

Our results suggest, that for applications, in which single molecules or monolayers are used, it is crucial to exactly know the molecular arrangement at the interface, because both, the orientation and the intermolecular bonding, can strongly influence the interface barrier height.

[1] M. Abel et al., ChemPhysChem 7:82 (2006)

DS 19.7 Wed 16:15 H 2013

Direct Optical Observation of Charge Transfer between Metals and Epitaxial Organic Layers — •Roman Forker, Giovanni Pizzi, Christian Golnik, Thomas Dienel, and Torsten Fritz — Institut für Angewandte Photophysik, Technische Universität Dresden, 01062 Dresden, Germany

We investigate epitaxial mono- and multilayers of 3,4,9,10-perylene tetracarboxylic dianhydride (PTCDA) *in situ* on various metal surfaces by a variant of optical absorption spectroscopy. During film growth we observe pronounced changes in the spectra.

Unlike on insulating substrates, such as mica [1], the 1 ML spectra on Au(100), Au(111), and Ag(111) are broad and essentially featureless. Detailed theoretical work for PTCDA/Au(111) suggested significant molecular level broadening and interface electron density rearrangement induced by the metal proximity [2], which might be applicable to Ag as well despite reports of gap states in that case [3]. In the second ML on these metals, however, our spectra exhibit monomeric character similar to the first ML on mica, which indicates weak interaction with the underlying PTCDA layer. Besides the monomeric part of the 2 ML spectra on Au, a new feature at around 2.0 eV appears. By comparison to K-doped PTCDA on mica (where the anion shows up at 1.85 eV) and to semi-empirical calculations we reason that we optically probe cationic PTCDA in the partly charged second ML on Au.

[1] H. Proehl *et al.*, Phys. Rev. Lett. **93** (2004), 097403.
[2] H. Vázquez *et al.*, Europhys. Lett. **65** (2004), 802.
[3] Y. Zou *et al.*, Surf. Sci. **600** (2006), 1240.

DS 19.8 Wed 16:30 H 2013

Hole injection barrier optimization at ITO/organic interfaces modified with strong molecular acceptors — •Ralf-Peter Blum[1], Benjamin Bröker[1], Steffen Duhm[1], Antje Vollmer[2], Ralph Rieger[3], Hans Joachim Räder[3], Klaus Müllen[3], Jürgen P. Rabe[1], and Norbert Koch[1] — [1]Institut für Physik, Humboldt-Universität zu Berlin, Newtonstrasse 15, D-12489 Berlin, Germany — [2]Berliner Elektronenspeicherring-Gesellschaft für Synchrotronstrahlung mbH, D-12489 Berlin, Germany — [3]Max Planck Institut for Polymer Research, Ackermannweg 10, D-55128 Mainz, Germany

The hole injection barriers at interfaces between N,N'-diphenyl-N,N'-bis(1-naphthyl)-1-1'biphenyl-4,4"diamine (α-NPD) and chemically modified ITO substrates have been studied by ultraviolet photoelectron spectroscopy (UPS). A decreased hole injection barrier was achieved by an appropriate arrangement of oriented dipoles, formed by chemisorption of strong electron acceptors, i.e., tetrafluoro-tetracyanoquinodimethane (F4-TCNQ) or hexacyanohexaazatriphenylene [HAT-(CN)]. In both cases thin acceptor layers induce coverage dependent work function shifts of more than 1 eV, thereby modifying the barrier to hole injection into α-NPD by up to 0.4 eV. We observed a linear dependence of the hole injection barrier versus the work function of modified ITO substrates. However, we find constant hole injection barriers for substrate work functions greater than 5.1 eV caused by localized states at the interface. This work is financially supported by the European Community project "IControl" (EC-STREP-033197).

DS 19.9 Wed 16:45 H 2013

Molecular band offsets and Charge Neutrality Levels at organic interfaces — •Héctor Vázquez[1], Mads Brandbyge[1], Antti-Pekka Jauho[1], and Fernando Flores[2] — [1]MIC-Department of Micro and Nanotechnology, Technical University of Denmark, DTU, DK-2800 Lyngby, Denmark. — [2]Departamento de Física Teórica de la Materia Condensada, Universidad Autónoma de Madrid, 28049 Spain.

We present a theoretical method to calculate the energy level alignment at interfaces of organic semiconductors based on the Charge Neutrality Levels (CNLs). The CNLs act as the electronegativity or effective Fermi level of the organic material at the interface.

We calculate the CNL position from the isolated organic molecule, rather than at the interface. We perform a DFT calculation of the molecule and consider energy corrections associated with the addition or removal of an electron; these result in shifts of the molecular levels, increasing the molecular gap with respect to DFT. The CNL position is calculated from the branch point of the molecular Greens function. The screening parameters at the interface, which also affect molecular level offsets, can be estimated from the static dielectric functions of the organic materials.

We have performed this analysis for several organic molecules, including, bathocuproine, Alq3 and hexaazatrinaphthylene derivatives, comparing induced dipoles and interface properties with experiment. Our work suggests that, at interfaces where the details of the interaction are not important, the CNL picture represents a general and intuitive model for understanding organic semiconductor interfaces.

DS 19.10 Wed 17:00 H 2013

Manipulation and Imaging of Aromatic Organic Molecules with Atomically Sharp Tips: The Last Atom Matters — Nicolae Atodiresei[1], Vasile Caciuc[2], Hendrik Hölscher[2], and •Stefan Blügel[1] — [1]Institut für Festkörperforschung,

Forschungszentrum Jülich, 52425 Jülich, Germany — [2]Center for NanoTechnology (CeNTech), University of Münster, Heisenbergstr. 11, 48149 Münster, Germany

The manipulation and imaging of organic molecules is of high interest for the development of nanoelectronic devices. Based on *ab initio* calculations we simulated how an aromatic organic molecule like benzene adsorbed on a Cu(110) surface can be imaged and mechanically manipulated in non-contact atomic force microscopy using two types of atomically sharp tips. A clean Silicon tip pushes the Benzene molecule from one adsorption site to another and can therefore be used for *lateral* manipulation processes. On the other hand, a Copper terminated tip binds to the benzene molecule lifting it from the Cu surface, thus leading to a *vertical* manipulation of this molecule.

DS 19.11 Wed 17:15 H 2013

Structure and electronic properties of mercaptoalkyl-ferrocenes, studies by STM — Lars Müller-Meskamp[1], •Silvia Karthäuser[1], Melanie Homberger[2], Ulrich Simon[2], and Rainer Waser[1] — [1]Institute of Solid State Research, Research Center Juelich GmbH, 52425 Juelich, Germany — [2]Institute of Inorganic Chemistry, RWTH-Aachen, Landoltweg 1, 52056 Aachen, Germany

The ability to access and use the electronic properties of individual molecules together with the inherent capability of self-organization, promises new possibilities for future microelectronic circuits. On this way the behavior of electroactive molecules with redox-centers, like ferrocenes, is especially interesting. Here we report on the structure and electronic properties of mercaptoalkyl-ferrocene self-assembled monolayers, studied by STM and STS. The molecular structures of pure full coverage and of submonolayer-coverage phases of different mercaptoalkyl-ferrocenes in mixed layers with alkanethiols on Au(111) are resolved. The ferrocenes form striped surface pattern resulting in equally spaced rows of ferrocene moieties. The obtained nanoscale lattice of functional groups offers an interesting potential for patterning of periodic structures. Besides this the electronic behavior of mercaptoalkyl-ferrocenes is studied by STS, which allows a direct determination of the decay constant of the ferrocene moiety.

References: [1] L. Müller-Meskamp et al., JoP: CS 61, 852 (2007). [2] L. Müller-Meskamp et al., PSS(a) 203, 1448 (2006).

DS 20: Organic Polymer-Metal Interfaces (SYSA 7)

Time: Wednesday 17:45–19:30 Location: H 2013

Invited Talk DS 20.1 Wed 17:45 H 2013

Designing the nanostructure of the organic polymer - metal interface — •Stephan V. Roth — HASYLAB at DESY, Notkestr. 85, D-22607 Hamburg, Germany

Thin film organic-metallic nanocomposites play an important role in biosensoring [1], solar cell applications [2] or organic electronics [3]. Depending on the desired application, one must tailor the interface metal - organic layer, e.g. selective contacting [4] or exploiting the plasmon resonances of the nanostructured metal layer [2,5,6]. Therefore, understanding the growth kinetics of the nanoparticle layer during deposition is of utmost importance to be able to design the nanocomposites' properties [6].

We exploited different deposition methods ranging from vacuum deposition [5,7] to solution casting [8] to install different metal layer morphologies. In combination with grazing incidence small-angle x-ray scattering we were able to observe the metal nanolayer growth kinetics on different organic and inorganic layers in real-time and present first results.

[1] B. Dubertret et al., Nat. Biotechnol. 19, 365 (2001)
[2] M. Westphalen et al., Sol. Energy Mater. Sol. Cells 61, 97 (2000)
[3] S. Gamerith et al., Adv. Funct. Mater. 17, 3111 (2007)
[4] T. L. Morkved et al., Appl. Phys. Lett. 64, 422 (1994)
[5] S.V. Roth et al., Appl. Phys. Lett. 88, 021910 (2006)
[6] A. Biswas et al., Vac. Techn. & Coat. 7, 54 (2006)
[7] S.V. Roth et al., Appl. Phys. Lett 82, 1935 (2003)
[8] S.V. Roth et al., Appl. Phys. Lett 91, 091915 (2007)

DS 20.2 Wed 18:15 H 2013

Photovoltaic effect in layer-by-layer self-assembled composite films of TiO_2 nanoparticles, polymers and quantum dots — •Rolf Kniprath[1], James T. McLeskey Jr.[2], Jürgen P. Rabe[1], and Stefan Kirstein[1] — [1]Humboldt University Berlin — [2]Virginia Commonwealth University, Richmond

We report on the properties of thin film hybrid photovoltaic devices with sensitized nanoporous TiO_2 anodes and polymeric hole transport layers (HTL). The TiO_2 films were grown with a layer-by-layer self-assembly process that relies on electrostatic interaction between inorganic particles and charged polymers. This method provides a simple means to incorporate sensitizer materials such as semiconductor quantum dots or light absorbing polymers during the film growth.

We fabricated two types of devices. One employs a novel, water-soluble polythiophene derivative which acts both as a sensitizer and as a HTL, the other uses strongly light absorbing CdTe and CdSe quantum dots as sensitizers and a highly conductive transparent polymer as a HTL. Both types of devices were grown on glass substrates coated with bilayers of transparent fluorine-doped tin oxide (FTO) and compact TiO_2. Evaporated gold electrodes served as back contacts. Current-voltage-measurements under white light and in the dark showed a pronounced photovoltaic effect for both systems and yielded photovoltages of up to 0.80V for the polythiophene devices and 1.1 V for the quantum dot devices.

DS 20.3 Wed 18:30 H 2013

Immobilization of nanoparticles on polymer brushes for nanosensors — •Smrati Gupta[1], Petra Uhlmann[1], Ulrich Oertel[1], Nikolai Gaponik[2], Alexander Eychmüller[2], and Manfred Stamm[1] — [1]Leibniz-Institut für Polymerforschung Dresden e.V., Hohe Strasse 6, 01069 Dresden, Germany — [2]Technische Universität Dresden, Physikalische Chemie-Elektrochemie, 01062, Dresden, Germany

We report on the immobilization of nanoparticles (Au, Ag or CdTe) on responsive polymer brushes by covalent or electrostatic interactions. Atomic force microscopy (AFM) was used to study the film morphology. The presence of nanoparticles on the polymer brushes was proved by X-ray photoelectron spectroscopy (XPS). Changes in optical properties of quantum dots/metal nanoparticles after the immobilization was studied by photoluminescence or UV-VIS spectroscopy. The exploitation of such polymer brushes revealed suppressed nanoparticle aggregation and facilitated complete surface coverage. Finally, the systems were used to fabricate nanosensors for solvents or for the pH of the surrounding aqueous medium. The concept is based on the variation of the photoluminescence with changing interparticle distance due to the swelling/deswelling of the responsive polymer brushes.

DS 20.4 Wed 18:45 H 2013

Near Infrared Sensitivity of PbS Quantum Dot Sensitized Organic Photodiodes — •Tobias Rauch[1,4], Michaela Böberl[1,2], Maksym Kovalenko[3], Sandro Tedde[1], Uli Lemmer[4], Jens Fürst[5], Wolfgang Heiss[3], and Oliver Hayden[1] — [1]Siemens AG, CT MM 1, D-91058 Erlangen, Germany — [2]CD Laboratory for Surface Optics, Universität Linz, A-4040 Linz, Austria — [3]Institute of Semiconductor and Solid State Physics, Universität Linz, A-4040 Linz, Austria — [4]Light Technology Institute, Universität Karlsruhe (TH), D-76131 Karlsruhe — [5]Siemens AG, MED RVV, D-91058 Erlangen, Germany

Composites of colloidal semiconductor quantum dots (QDs) and semiconducting polymers expand the sensitivity of organic photodetectors beyond the visible spectrum (> 780 nm).

Blending the photoactive P3HT:PCBM layer of our bulk heterojunction photodetectors with near-infrared sensitive PbS QDs pushes the spectral response of the detector up to wavelengths of 1500 nm. The QDs show a photoconductive gain linearly increasing with the bias voltages. At 1300 nm, the photodetectors yield external quantum efficiencies of 8% remaining constant over more than 3 decades of irradiation intensity. Good signal-to-noise ratios can be achieved for signals up to 10 kHz.

The sensitization of organic photodetectors with colloidal QDs enables organic optolectronics to enter the field of IR related applications like IR imaging, security sensing and scanning.

DS 20.5 Wed 19:00 H 2013

Interface engineering and advanced photon harvesting in organic solar cells — •Robert Koeppe[1], Pavel A. Troshin[2], Rimma N. Lyubovskaya[2], and N. Serdar Sariciftci[1] — [1]Linz Institute for Organic Solar Cells (LIOS), JKU Linz — [2]Institute of Problems of Chemical Physics, Russian Academy of Science, Chernogolovka

We consider two approaches towards increasing the photon harvesting in low energy gap organic solar cells. These devices usually have a low absorption cross section in the blue and green part of the spectrum, which decreases the quantum efficiency in this range. Both approaches require a tuning of the interfaces between the active materials in the device. Firstly, we use the complexing of a pyrrolidinofullerene with pendant pyridil groups to zinc-phthalocyanine to specifically organize the interfaces in a multicomponent organic solar cell. [P.A. Troshin et al., Chem. Mater. 19, 5363 (2007)] Secondly, we consider the use of CdSe/ZnS semiconductor nanocrystals as energy transfer donors that channel the energy from the absorbed light onto the active material of the solar cell. Here, the ligand shell around the nanocrystals plays an important role to insulate the crystals and still allow energy transfer. The dependence of the energy transfer efficiency on the length of the ligands is determined and a photodiode device made of zinc-phthalocyanine is presented, where the addition of CdSe/ZnS nanocrystals lead to an enhanced sensitivity in the green spectral region. [R. Koeppe et. al., Sol. Energ. Mat. Sol. Cells 91(11), 986 (2007)]

DS 20.6 Wed 19:15 H 2013

In-Situ Investigations of Si/Polypyrrole Interfaces by Pulsed Photoluminescence and IR Spectroscopic Ellipsometry — •Carl Matthias Intelmann[1], Vitali Syritski[2], Karsten Hinrichs[3], and Jörg Rappich[1] — [1]Hahn-Meitner-Institut Berlin GmbH, Department Silicon Photovoltaics (SE1), Berlin, Germany — [2]Tallinn University of Technology, Department of Materials Science, Tallinn, Estonia — [3]ISAS - Institute for Analytical Sciences, Department Berlin, Germany

Conducting polymers - such as polypyrrole (PPy) - offer a unique combination of properties, which are interesting for photovoltaic applications. Important - especially - for solar cells is a low recombination rate of charge carriers at the silicon interfaces, which can be inspected by the band gap related photoluminescence (PL). We used pulsed PL techniques to investigate the recombination behaviour at the Si/PPy interface. The PPy films were directly deposited on Si substrates by electrochemical methods.

Our ex-situ and in-situ PL investigations show that PPy films on Si surfaces lead to well passivated Si interfaces. Ex-situ infrared spectroscopic ellipsometry (IR-SE) measurements yielded a thickness of approx. 45 nm of the ultrathin PPy films. Additionally performed in-situ IR-SE measurements show negligible formation of SiO_x species at the Si/PPy interface.

DS 21: High-k Dielectric Materials - Synthesis, Properties, Applications

Time: Wednesday 14:30–16:30 Location: H 2032

Invited Talk DS 21.1 Wed 14:30 H 2032

Challenges and Chances with new materials in semiconductor device applications — •Stefan Jakschik and Karl-Heinz Küsters — Qimonda Dresden GmbH & Co. OHG, Königsbrücker Strasse 180, 01099 Dresden, Germany

With entering sub 50nm nodes transistor scaling is leaving the era of traditional scaling and performance gain as well as miniaturization is achievable only by introducing further innovative performance boosters. A continuous key question of scaling is leakage control and voltage scaling which is answered nowadays by introducing materials with a high dielectric constant in MOS transistors, DRAM capacitors and FLASH storage devices. Opening the integration choice to new materials gives the chance to choose the effective oxide thickness and the work-function according to specific device requirements. On the other hand many new questions have to be answered.

We will show ways to design the threshold voltage of MOS devices with the right material choice, highlighting here Hf-oxide and scaled silicon oxide based systems with Titanum and Tantalum containing electrodes. Special attention is given to channel design options like fluorine and nitrogen implants as well as silicon germanium quantum wells. Investigating more thoroughly the dielectric, traps and charges has to be taken into account. These influence the leakage current as well as the reliability of the devices. Especially FLASH devices have a rigid leakage requirement though scaling is driving the application of high dielectric constant materials here as well. Among others Aluminiumoxide and Dysprosiumoxide based solutions are presented.

Invited Talk DS 21.2 Wed 15:00 H 2032

Are Optical Measurements Sensitive to Quantum Confinement? — •Alain Diebold — College of Nanoscale Science and Engineering, Albany, NY USA

Nanofabrication methods have produced ultra-thin films, nanowires of various cross-sectional shapes, and quantum dots. Characterization of nano-scale materials has proven the existence of quantum confinement or quantum size effects (QSE). Of note to the characterization community is observation of QSE in thin metal films using X-ray Photoelectron Spectroscopy. This presentation emphasizes optical observation of quantum confinement in ultra-thin silicon semiconductor films. The first step in identifying changes in optical properties, especially the dielectric function, is demonstrating that the data is not due to other phenomena such as stress. We show that the blue shift E1 critical point of thin silicon on insulator films is not due to stress. This blue shift is attributed to quantum confinement. We also discuss why energy shifts in E1 smaller than KT can be observed optically.

DS 21.3 Wed 15:30 H 2032

Broadband dielectric response of $CaCu_3Ti_4O_{12}$: significant intrinsic properties — •Stephan Krohns[1], Christian Kant[1], Torsten Rudolf[1], Franz Mayr[1], Peter Lunkenheimer[1], Stefan Ebbinghaus[2], and Alois Loidl[1] — [1]Experimental Physics V, Center for Electronic Correlations and Magnetism, University of Augsburg, 86135 Augsburg, Germany — [2]Solid State Chemistry, Universitiy of Augsburg, 86135 Augsburg, Germany

For applications, e.g., in wireless electronics, materials with colossal dielectric constant are in great demand. Since first reports of very large ("colossal") dielectric constants ϵ' up to the order of 10^5 in $CaCu_3Ti_4O_{12}$ (CCTO), this material is in the focus of scientific and technical interest [1,2]. Not only the understanding of the origin of the most likely extrinsic colossal ϵ' values is important, but also the clarification of the intrinsic dielectric properties is of high relevance. By combining dielectric and optical methods, we provide dielectric spectra of CCTO covering 15 decades in frequency. Aside of its colossal dielectric constant, CCTO behaves unusual also in other respects. For example, we report an unusual temperature dependence of the low lying phonon modes, revealing a softening that may point to an underlying ferroelectric instability in this material. In addition, information on electronic excitations in CCTO is provided [3].

[1] C.C. Homes et al., Science 293, 673 (2001). [2] S. Krohns et al., Appl. Phys. Lett. 91, 022910 (2007). [3] Ch. Kant et al., arXiv:0709.1065

DS 21.4 Wed 15:45 H 2032

Modelling a nanoscale ferroic OFET — •Sibylle Gemming[1], Gotthard Seifert[2], Andrey Enyashin[2] und Lukas M. Eng[3] — [1]Forschungszentrum Dresden-Rossendorf, D-01314 Dresden, Germany. — [2]Fachbereich Chemie, Technische Universität Dresden, D-01062 Dresden, Germany. — [3]Institut für Angew. Physik und Photophysik, Technische Universität Dresden, D-01062 Dresden, Germany.

The present study describes an approach for the scale-bridging modelling of ferroic materials as functional elements in micro- and nanoelectronic devices. Ferroic materials are characterised by temperature-dependent complex ordering phenomena of the internal magnetic, electronic, and structural degrees of freedom with several involved length and time scales. Hence, the modelling of such compounds is not straighforward, but relies on a combination of electronic-structure-based methods like ab-initio and density-functional schemes with classical particle-based approaches given by Monte-Carlo simulations with Ising, lattice-gas, or Heisenberg Hamiltonians, which incorporate material-specific parameters both from theory and experiment. The interplay of those methods is demonstrated for device concepts ba-

sed on electroceramic materials like ferroelectrics and multiferroics, whose functionality is closely related with their propensity towards structural and magnetic polymorphism. In the present case, such scale-bridging techniques are employed to aid the development of an organic field effect transistor on a ferroelectric substrate generated by the self-assembly of field-sensitive molecules on the surfaces of ferroic oxides.

DS 21.5 Wed 16:00 H 2032

Molecular beam deposition of $LaLuO_3$ thin films with high dielectric constant and low leakage current — •J. M. J. Lopes, U. Littmark, M. Roeckerath, St. Lenk, J. Schubert, and S. Mantl — Institute of Bio- and Nanosystems and Center of Nanoelectronic Systems for Information Technology, Research Centre Juelich, D-52425 Juelich, Germany

Although the introduction of hafnium-based high-κ dielectrics in the next CMOS generation has been announced, the implementation of materials with a dielectric constant even higher than 20 will be required in order to satisfy the future demands in CMOS applications. In this contribution, we report on lanthanum lutetium oxide, a ternary rare-earth based material that has recently appeared as a promising candidate[1]. $LaLuO_3$ thin films were grown on (100) Si substrates by molecular beam deposition and electrically characterized by capacitance-voltage (C-V) and current-voltage (I-V) measurements. Additionally, a combination of characterization methods such as Rutherford backscattering spectrometry, transmission electron microscopy, X-ray reflectometry, and X-ray diffraction were used to study their composition and microstructural characteristics. We will present results of a systematic investigation on the film preparation, which allowed the deposition of $LaLuO_3$ thin films with EOT $\leq$ 1.5 nm, low leakage current densities of about 5 mA/cm^2 at -1 V gate bias, and higher κ-values around 30.

[1] J. M. J. Lopes et al. Appl. Phys. Lett. 89, 222902 (2006).

DS 21.6 Wed 16:15 H 2032

Preparation, morphology and physical properties of nano-$Ln_{1*x}Sr_xMnO_3$ perovskites — •Rafal J. Wiglusz[1], Wieslaw Strek[1], Dariusz Hreniak[1], Glikeria Kakali[2], Anna Gaki[2], and Miroslaw Miller[3] — [1]Institute of Low Temperature and Structure Research, Polish Academy of Sciences,, ul. , Okolna 2, 50-422 Wrocław, Poland — [2]Chemical Engineering Department National Technical University of Athens 9 Heroon, Polytechniu Str., 15773 Athens, Greece — [3]Chemical Department, Wroclaw University of Technology, Wybrzeze Wyspianskiego 27, 50-370 Wroclaw, Poland

The nano-$Ln_{1*x}Sr_xMnO_3$ perovskites (where Ln is La, Sm or Tb) are the important materials for the Solid Oxide Fuel Cells (SOFC). In present work, the glycine/nitrate powder synthesis has been described using a unique combination of metal nitrates and glycine stoichiometrically, which produces nano-particles. The obtained nano-powders have been characterized by X-Ray Diffraction (XRD) and Transmission Electron Microscopy (TEM) studies. The effect of grain sizes of nano-crystallites on the optical, magnetic and electrical properties has been studied and discussed.

DS 22: High-k Dielectric Materials - Synthesis, Properties, Applications

Time: Wednesday 16:45–18:30 Location: H 2032

Invited Talk DS 22.1 Wed 16:45 H 2032

Development of novel processes for atomic layer deposition of high-k dielectrics — •Jaakko Niinistö, Kaupo Kukli, Mikko Ritala, and Markku Leskelä — Laboratory of Inorganic Chemistry, Department of Chemistry, P.O. Box 55, FI-00014 University of Helsinki, Finland

Atomic layer deposition (ALD) has gained considerable interest in the recent years as a thin film deposition method to overcome many technological problems faced by the semiconductor industry. Deposition of high-k materials for CMOS and DRAM applications are the main application areas for ALD.

The success of ALD is built on chemistry. The unique characteristics of ALD can be achieved and benefited only with precursors that provide the self-limiting film growth through the saturative surface reactions. For high-k materials the leading solutions include the oxides of Hf and Zr. For ALD of these materials, alkylamides have gained wide interest as precursors. However, thermal decomposition of the alkylamides at rather low temperatures prevent the ALD-type growth mode. The need for process development and existing ALD processes of ZrO2 and HfO2 with recent advancements are discussed.

In this presentation, recent research with cyclopentadienyl-precursors, which offer high thermal stability, is reviewed. In addition, we introduce mixed alkylamido-cyclopentadienyl precursors of Zr and Hf. With ozone as the oxygen source, the process yields ZrO2 films with high permittivity cubic phase and low leakage current density. Finally, results of doping the ZrO2 and HfO2 films are presented.

Invited Talk DS 22.2 Wed 17:15 H 2032

Towards a better understanding of the dielectric collapse in high-K BST thin film capacitors — •Regina Dittmann[1], Rafael Plonka[2], Nikolay Pertsev[3], Susanne Hoffmann-Eifert[1], and Rainer Waser[1,2] — [1]Institut für Festkörperforschung, Forschungszentrum Jülich, 52425 Jülich — [2]Institut für Werkstoffe der Elektrotechnik, RWTH Aachen, 52056 Aachen — [3]A. F. Ioffe Physico-Technical Institute, 194021 St. Petersburg, Russia

According to permittivities in the order of 10.000 observed in bulk ceramic samples, the perovskite material BaxSr1-xTiO3 (BST) is a promising candidate for future DRAM storage capacitors. A considerable drawback is that in polycrystalline thin films, the permittivity collapses to values in the order of 100 and decreases strongly with decreasing thickness. We addressed the influence of defects, substrates-imposed strain and the electrode interfaces on the dielectric collapse by investigating fully epitaxial SrRuO3/BST/SrRuO3 thin film capacitors. High resolution transmission electron microscope investigations prove the SrRuO3-BST interfaces to be atomically sharp and free of any defective "dead-layers". These capacitors exhibit bulk-like permittivity in the order 4000 and their thickness dependence can be well described by an extended Ginzburg-Landau-Devonshire model by taking into account plastic strain relaxation in BST thin films and finite screening of depolarizing fields by the SrRuO3 electrodes. We will compare the data to thin film capacitors with noble metal electrodes and discuss which type of interface is superior in terms of its screening ability.

DS 22.3 Wed 17:45 H 2032

From hexagonal Pr2O3 films to lattice matched twin-free PrO2/Si(111) with cubic structure — Thomas Weisemoeller, Andreas Greuling, Sebastian Gevers, Carsten Deiter, and •Joachim Wollschläger — Fachbereich Physik, Universität Osnabrück, Barbarastr. 7, 49069 Osnabrück, Germany

Praseodymiumoxide is a well suited material for epitaxial high-k films on Si due to both its high dielectric constant (k=25-30). Oxide films deposited by molecular beam epitaxy (MBE) on Si(111) have Pr2O3 stoichiometry with metastable hexagonal structure[1]. It is well known that these films can be transformed into a (less lattice matched) cubic phase by annealing at low oxygen pressure [2]. Here we present experiments performed after annealing Pr2O3 films with hexagonal structure at high oxygen pressure. The crystal structure of these films has been investigated by synchrotron based x-ray diffraction (XRD) including grazing incidence (GIXRD). The oxide films have fluorite structure which points to the formation of PrO2 with cubic structure which matches the Si lattice in all directions. The PrO2 films are exclusively B-oriented so that no twins are formed. The structure of both the oxide films and the interface has been investigated by crystal truncation rod (CTR) analysis. Depending on the preparation the oxides films show some oxygen deficiency. In addition, silicate layers are formed at the interface as verified by both XRD and x-ray reflectometry (XRR).

[1] E.J. Tarsa et al., Appl. Phys. Lett. 63 (1993) 539.
[2] T. Schroeder et al., J. Appl. Phys. 99 (2006) 014101.

DS 22.4 Wed 18:00 H 2032

Structural, chemical and electrical characterization of HfNO-HfTiO high-k dielectric stack — Visorian Mikhelashvili[1], Gadi Eisenstein[1], Thangadurai Paramasivam[2], and •Wayne Kaplan[2] — [1]Electrical Engineering Dept. Technion — [2]Material Engineering Dept.Technion

We study the influence of annealing temperature on structural, compositional and electrical characteristics of a MOS structure with a high-k dielectric based on a 5 nm HfNO-HfTiO nanolaminate stack. A common feature of all samples independent on annealing temperature is the observation of two distinct ˜2-2.5 and 2.3-2.5 nm thick layers, respectively for transition (close to Si substrate) and top layers. The transition layer is amorphous, while in the top layer some crystalline inclusions embedded into the amorphous matrix are observed. EDS line-scans and XPS analysis showed that the transition layer is similar to metal-Si-O-N or metal-Si-O. The minimum values of quantum mechanical corrected Effective Oxide Thickness close to 1.29 and 0.86 nm, respectively for structures with Au and Cr electrodes. A large reduction of leakage current density to 1.5X10-8 and 2.9X10-7 A/cm2, respectively for Au and Cr gate electrodes at an electric fields of 2 MV/cm was observed with annealing temperature and breakdown electric filed as high as ˜10-12 MV/cm, was measured independently of the electrodes type.

DS 22.5 Wed 18:15 H 2032

Photoemission and absorption spectroscopy for in situ investigations of the ALD growth — •Massimo Tallarida[1], Konstantin Karavaev[1], Dieter Schmeisser[1], and Ehrenfried Zschech[2] — [1]Brandenburgische Technische Universität Cottbus, Konrad-Wachsmann-Allee 17, 03046 Cottbus, Germany — [2]AMD Saxony LLC & Co. KG, Center for Complex Analysis, Wilschdorfer Landstr. 101, D-01109 Dresden, Germany

We have investigated the growth of Hf-oxide on Si by means of photoemission and X-ray absorption spectroscopy using synchrotron radiation at Bessy, Berlin. The Hf-oxide layers were grown via atomic layer deposition (ALD) using an in-situ ALD reactor attached to the investigation chamber. The XPS and XAS spectra were measured after every deposition cycle by transferring the sample into the investigation chamber without breaking the vacuum. From the experimental data we have obtained information about the early stages of the Hf-oxide growth, concerning in particular the reactivity of the interface with Si. Due to the possibility to study the layers after every cycle and with different oxidation parameters without exposing them to contaminants, the in situ investigation revealed to be a very important method to understand the growth properties of Hf-oxide.

DS 23: High-k Dielectric Materials - Synthesis, Properties, Applications
The posters can also be presented at Poster A on Tuesday morning (DS poster session).

Time: Wednesday 18:30–20:30 Location: Poster C

DS 23.1 Wed 18:30 Poster C

Leakage current in high-k thin film capacitor stacks — •Herbert Schroeder — IEM im Institut für Festkörperforschung und CNI, Forschungszentrum Jülich GmbH, D-52425 Jülich

High-permittivity thin insulating films of the perovskite-type mixed-oxides such as $SrTiO_3$ or (Ba,Sr)TiO_3 are candidates as capacitor dielectrics in advanced DRAM cells and as new gate materials in MOSFETs (see ITRS Roadmap). One of the most important issues for these applications is a sufficiently low leakage current to avoid malfunction of the devices. Although a large number of experimental data on leakage through metal-insulator-metal (MIM) thin film capacitor structures is published for perowskite-type mixed oxides, the mechanistic interpretation is quite inconsistent. In this contribution the experimental data will be compared to simulation studies for an advanced leakage current model combining the electronic carrier injection/ejection at the electrode interfaces (described by thermionic emission) with the film conduction properties of the thin dielectric film (modelled as wide band gap semiconductor). Many parameters are varied: Besides the externally given electric field, dielectric thickness and temperature, these are the usually unknown defect properties [type (donor, acceptor), concentration and in-gap energy level as well as type and degree of compensation] and that of the electrode interfaces. From the resulting trends guidelines for a low leakage MIM stack with high effective permittivity are extracted.

DS 23.2 Wed 18:30 Poster C

Induced Ferroelectricity in Strained Epitaxial $SrTiO_3$ Films on Various Substrates — Eugen Hollmann, Jürgen Schubert, Rolf Kutzner, and •Roger Wördenweber — Institut für Bio- und Nano-Systeme and cni, Forschungszentrum Jülich, D-52425 Jülich

Thin films of ferroelectric materials ($SrTiO_3$, (Ba,Sr)TiO_3 and others) are currently being used to develop active microwave devices (phase shifters, tunable high-Q resonators or filters) for cryogenic and room temperatures operation. In this contribution, the impact of strain on structure and ferroelectric properties of epitaxial $SrTiO_3$ films on various substrate materials - substrates with larger ($DyScO_3$) and smaller ($NdGaO_3$ and CeO_2/Al_2O_3) in-plane lattice constant, respectively - is analyzed. It is demonstrated that the mismatch of the lattices or, alternatively, the mismatch of the thermal expansion coefficients of films and substrate impose biaxial compressive or tensile strain to the $SrTiO_3$ films, respectively. The strain leads to a small tetragonal distortion of the $SrTiO_3$ lattice and has a large impact of the ferroelectric properties of the films. With decreasing film thickness and at low temperatures the permittivity deviates from the *classical* Curie-Weiss behavior. The thinnest sample shows an enhancement of the dielectric constant at room temperature by up to a factor of 3. Furthermore, strain induced ferroelectricity is observed which agrees with theoretical predictions. For electric fields parallel to the film surface induced ferroelectricity is observed for $SrTiO_3$ that is exposed to in-plane tensile strain, i.e., ferroelectricity is observed for temperatures up to 210 K and 325 K for strained $SrTiO_3$ on $CeO_2/Al2O_3$ and $DyScO_3$, respectively.

DS 23.3 Wed 18:30 Poster C

Solvothermal sol-gel process for synthesis of $Ba_{0.5}Sr_{0.5}TiO_3$ — •Dirk Spitzner[1], Emanuel Gutmann[1], Boris Mahltig[2], and Dirk C. Meyer[1] — [1]TU Dresden, Institut für Strukturphysik, 01062 Dresden — [2]Gesellschaft zur Förderung von Medizin-, Bio- und Umwelttechnologien, GMBU e.V., Department: Functional Coatings, Postfach 520165, 01317, Dresden

In the solid solution of barium strontium titanate (BST) the transition temperature from the paraelectric to ferroelectric phase and hence the electrical properties can be tuned over a wide range, what is of interest for various electronic applications. Beside vacuum deposition methods, thin films of BST can be synthesized by chemical solution deposition. We modified a classic sol-gel deposition process using barium-, strontium-acetate and titanium-isopropoxide as precursor in acetic acid and acetylacetone by introducing a solvothermal treatment of as-synthesized sols. The decomposition and crystallization behaviour in the resulting powders and films were analyzed by thermal analysis (TG, DTA), X-ray diffraction and X-ray reflectometry. In comparison to untreated sols a different transition behaviour is observed when the sols are prepared by using a solvothermal procedure.

DS 23.4 Wed 18:30 Poster C

Band gap determination of thin Praseodymiumoxide layers on Aluminiumoxynitride films — •Matthias Bergholz and Dieter Schmeisser — Brandenburgische Technische Universität Cottbus, Angewandte Physik - Sensorik, Konrad-Wachsmann-Allee 17, 03046 Cottbus, Germany

High-k dielectrics are important as never bevore in semiconductor industry. We investigate Pr_2O_3 as one representative of this group on Silicon and Silicon-Aluminium oxynitride substrates. In earlier work we observed the positive influence of this AlO_xN_y intermediate layer on the electrical properties of the Pr_2O_3 layer. Now we present in-situ EELS, XPS and UPS measurements of gradually grown thin Pr_2O_3 on AlO_xN_y. From these measurements we determine the band structure and find a very fast change of the band gap for the first few Ångström, coupled with n-type behaviour for the Pr_2O_3 film. These results are compared with RIXS measurements of a 5 nm Pr_2O_3 on a 1 nm thick AlO_xN_y layer.

DS 23.5 Wed 18:30 Poster C

X-ray photoemission spectroscopy of Aluminium Oxynitride on Si(001) and the rise as buffer layers — •Yevgen Burkov,

Karsten Henkel, and Dieter Schmeisser — BTU Cottbus, Angewandte Physik - Sensorik, Konrad-Wachsmann-Allee 17, 03046 Cottbus, Germany

Praseodymium oxide (Pr_xO_y) is one of the candidate as high-k transistor gate dielectrics, but aluminium oxynitride (Al_xON_y) as buffer layer is needed to prevent diffusions from the silicon into Pr_xO_y and to hinder charge injection from the semiconductor into the insulator. The thermal stability and thickness dependence of aluminum oxynitride (Al_xON_y) has been investigated by synchrotron radiation photoemission spectroscopy (SR-PES). Al_xON_y layers were prepared by low energy ion-beam assisted deposition (LE-IBAD) at room temperature on a silicon substrate cleaned with HF-acid. Aluminium oxynitride is stable till 800°C. From photoemission spectra we can assess that silicon oxynitride is built as first and then the growth of Al_xON_y follows. Resonant inelastic X-ray scattering measurements with synchrotron radiation have been performed. The combination of X-ray absorption spectroscopy (XAS) and RIXS make possible to determinate the band gap of Al_xON_y.

DS 23.6 Wed 18:30 Poster C

Unified approach for the calculation of direct and Fowler-Nordheim tunneling current in multi-layered high-k gate dielectric stacks — •Mahyar Boostandoost, Ebrahim Nadimi, and Christian Radehaus — Technische Universität Chemnitz Fakultät für Elektrotechnik und Informationstechnik Professur für Opto- und Festkörperelektronik 09107 Chemnitz

A quantum mechanical model is developed to compute the tunneling current in the p-MOSFET, with multi-layered high-k gate stacks. A unified approach is applied to the calculation of direct and Fowler-Nordheim tunneling regimes. The model uses self-consistent approach, based on a numerical solution of the coupled Schrödinger and Poisson equations and an open boundary condition at dielectric/gate interface. The tunneling current will be derived using the lifetime of electrons in the quasi-bound states. The gate tunneling current of different high-k stacks including HfO_2, ZrO_2, Si_3N_4 and an intefacilal SiO_2 layer are compared. For a given equivalent oxide thickness, the gate leakage current decreases by increasing the high-k dielectric thickness or by decreasing the interlayer thickness. Crossing point in the I-V curves at high gate biases are observed for all gate stacks. We also investigate the influence of the effective mass on the tunneling current and presented the results considering different possible situations.

DS 23.7 Wed 18:30 Poster C

Tunneling effective mass in ultrathin silicon oxynitride gate dielectrics — •Ebrahim Nadimi[1], Christian Golz[2], Martin Trentzsch[2], Lukas Herrman[2], Karsten Wieczorek[2], and Christian Radehaus[1] — [1]Technische Universität Chemnitz, Fakultät für Elektrotechnik und Informationstechnik, Reichenhainer Str. 70, D-09126 Chemnitz, Deutschland — [2]AMD Saxony LLC & Co. KG, Wilschdorfer Landstraße 101, D-01109 Dresden, Deutschland

In this work we study the dependence of the tunneling effective mass of electrons on gate dielectric nitrogen concentration and thickness in metal-oxide-semiconductor field-effect-transistors (MOSFETs) with lightly doped silicon oxynitride (SiOxNy) gates. The dependences of the effective mass on nitrogen concentration and dielectric thickness are extracted by fitting the computation results for the gate leakage current to the experimental data measured by us for samples with different thicknesses and nitrogen concentrations. The direct tunneling current is modeled by applying a Schrödinger-Poisson solver with one-side-open boundary condition. Nitrogen concentration and thickness of samples are determined using X-Ray photoemission spectroscopy (XPS). The obtained results show a strong dependence of the effective mass on the sample thicknesses and nitrogen concentration. The electron effective mass is found to increase as the thickness decreases and the higher nitrogen concentration causes a reduction in effective mass.

DS 23.8 Wed 18:30 Poster C

Optical characterization of HfO_2-based high-k gate stacks — •Martin Weisheit, René Hübner, Hans-Jürgen Engelmann, Inka Zienert, Susanne Ohsiek, Kornelia Dittmar, Michael Hecker, Martin Trentzsch, and Ehrenfried Zschech — AMD Saxony LLC & Co. KG, Wilschdorfer Landstraße 101, 01109 Dresden

HfO_2 is currently introduced as a high-k gate dielectric into large scale semiconductor production of logic devices. Along with HfO_2, a number of other new materials will have to be introduced into the gate stack, namely ultrathin work function layers and metal gates. This results in a complex gate stack that challenges traditional characterization techniques. In this presentation we demonstrate how a combination of complementary methods allows quantitative determination of relevant parameters. Important information can be derived from the optical properties of the stack - such as the bandgap of the HfO_2 - which are measured by Variable Angle Spectroscopic Ellipsometry (VASE). However, due to the very thin individual layers of the stack, independent determination of thickness and refractive index is difficult. Therefore, TEM and X-Ray Reflectivity are needed as complementary methods for an accurate measure of the layer thicknesses. Using the Drude model, VASE is then employed to characterize the electrical conductivity of the TiN metal gate layers, which is compared to Microscopic Four-Point Probe measurements and discussed with respect to chemical composition as determined by XPS and Auger electron spectroscopy. The work described in this presentation has been funded in line with the technology funding for regional development (ERDF) of the European Union and by funds of the Free State of Saxony.

DS 23.9 Wed 18:30 Poster C

Diagnostics of electrical surface parameters using conductive and electrostatic force microscopy — •Teodor Gotszalk[1], Grzegorz Wielgoszewski[1], Ehrenfried Zschech[2], and I. W. Rangelow[3] — [1]Wroclaw University of Technology, Faculty of Microsystem Electronics and Photonics, ul. Janiszewskiego 11/17, 50-372 Wroclaw, Poland — [2]AMD Saxony LLC & Co., Wilschdorfer Landstr. 101, D-01109 Dresden, Germany — [3]Technical University of Ilmenau, Gustav-Kirchoff-Strasse 1, D- 98 693 Germany

Failure analysis and reliability investigations of high-κ dielectrics films for the MOSFET transistors (e.g. silicon oxynitride or Hf oxide) films very often require high-resolution local measurements of electrical surface parameters. This kind of experiments can be performed using conductive atomic force microscopy, which provides simultaneous measurement of surface topography and current flowing through the investigated layer. In our experiments a precise measurement and control scanning probe system, which integrated a DC and AC low-noise current-to-voltage converter of picoampere resolution enabling high resolution of electrical conductance and capacitance in wide frequency range, was applied. In this presentation we will describe the architecture of the designed and applied experimental set-up. In addition we will also present results of simultaneous measurements of topography and tunneling current on silicon oxynitride ultra-thin films of different thickness and different composition, but also results of test measurements on highly oriented pyrolytic graphite (HOPG). We will also describe the possible usage of scanning electrostatic force microscopy, which in our opinion enables quantitative measurements of electrical voltages on the investigated surface of the microelectronic circuits and materials. In these experiments we applied near-field sensors with integrated piezoresistive and piezoelectrical deflection. In this way we simplified the architecture of the measurement system and enabled new applications on technological samples. In our talk we will describe the metrological properties of the applied sensors and instrumentation.

DS 23.10 Wed 18:30 Poster C

Fully depleted SOI-nMOSFETs with Gadolinium scandate as high-κ dielectric. — •M. Roeckerath[1], J. M. J. Lopes[1], T. Heeg[2], J. Schubert[1], and S. Mantl[1] — [1]Institute of Bio- and Nanosystems and Center of Nanoelectronic Systems for Information Technology, Research Centre Juelich, D-52425 Juelich, Germany — [2]Department of Materials Science and Engineering, The Pennsylvania State University, University Park, Pennsylvania 16802-5005, USA

Rare earth scandates are a promising class of materials as alternative high-κ gate dielectrics for future CMOS applications due to their good morphological and electrical properties (D. G. Schlom et. al., MRS Bull. 27, 198 (2002)). In particular, gadolinium scandate has recently attracted increasing attention since it exhibits a high thermal stability, a sufficiently large κ-value of ∼23 and is in contrast to other rare earth oxides not hygroscopic. In this work long channel n-metal-oxide-semiconductor field-effect transistors (nMOSFETs) on thin SOI (∼25 nm) have been prepared with gadolinium scandate as high-κ gate dielectric and a TiN metal gate in a gate last process. The $GdScO_3$ films were deposited by electron beam evaporation from a stoichiometric ceramic target in high vacuum conditions. Prior to the deposition different surface treatments of the substrates were applied to vary the interface conditions. Readily fabricated devices were electrically characterized by DC-measurements. They reveal well behaved output and transfer characteristics with high I_{on}/I_{off} ratios of 10^6-10^8 and steep

inverse subthreshold slopes of ∼66 mV/dec. Carrier mobilities comparable to other high-k dielectrics of ∼150 cm^2/Vs were determined.

DS 23.11 Wed 18:30 Poster C

XRD/GIXRD studies of Praseodymium Oxide on Si(111) — •Andreas Greuling[1], Thomas Weisemöller[1], Carsten Deiter[1], Joachim Wollschläger[1], and Thomas Schröder[2] — [1]Universität Osnabrück, Barbarastr. 7, D-49069 Osnabrück, Germany — [2]IHP-Microelectronics, Im Technologiepark 25, D-15236 Frankfurt(Oder), Germany

Praeseodymium sesquioxides ($\epsilon \approx 25$) are well suited for epitaxy on Si based technologies since several crystalline phases are lattice matched to Si substrates. It is known that one can deposit metastable hexagonal Pr_2O_3 on Si(111)[1] which can be transformed to the cubic Pr_2O_3 phase due to annealing with a low oxygen pressure. Here, we present CTR-Analysis of thin Praseodymium Oxide films (5nm/10nm) on Si(111)[2]. The Praseodymium Oxide was deposited on Si(111) at 625°C. Following epitaxy the h-Pr_2O_3/Si(111) samples were annealed at 10^5 Pa O_2. After that ex situ XRD and GIXRD experiments were performed at HASYLAB(DESY). We developed a simulation program which allows us to compute the intensity of a CTR using experimental data in order to fit the parameters of the underlying model. During our work we compared simulation runs of h-Pr_2O_3, c-Pr_2O_3 and PrO_2 on Si(111). Using our program for CTR-analysis we checked models with single phases and phase mixtures.

[1] H.J. Osten, J.P. Liu, E. Bugiel, H.J. Müssig, and P. Zaumseil, J. Cryst. Growth 235, 229 (2002).

[2] Samples were prepared at IHP.

DS 23.12 Wed 18:30 Poster C

In-situ ALD growth of Hafnium oxide films — •Konstantin Karavaev[1], Massimo Tallarida[1], Dieter Schmeisser[1], and Ehrenfried Zschech[2] — [1]Brandenburgische Technische Universität Cottbus, Angewandte Physik - Sensorik, Konrad-Wachsmann-Allee17, 03046 Cottbus, Germany — [2]AMD Saxony LLC & Co. KG, Center for Complex Analysis, Wilschdorfer Landstr. 101, D-01109 Dresden, Germany

We report on a novel system for in-situ atomic layer growth (ALD) of high-k dielectric films. First results were obtained for Hf-oxide samples by using Hf-tetrachloride as precursor and water as oxidizer. We compare the photoelectron spectra of Si2p, O1s and Hf4f of our in-situ prepared films with samples (ex-situ) prepared by industrial ALD reactors and discuss similarities and differences observed in the core level spectra of the various samples by considering the different growth conditions.

DS 24: Trends in Ion Beam Technology: From the Fundamentals to the Application

Time: Thursday 9:30–11:00 Location: H 2013

Invited Talk DS 24.1 Thu 9:30 H 2013

Nanostructures produced with energetic heavy ion projectiles — •Christina Trautmann — Gesellschaft für Schwerionenforschung, Planckstr. 1, 64291 Darmstadt, Germany

Heavy ions of kinetic energies in the MeV to GeV range offer unique possibilities of modifying materials properties and producing micro and nanostructures. Each projectile creates a cylindrical track with a few nanometers in diameter, consisting of physically and chemically modified material. The small track size in combination with the large ion range (up to 100 μm and more) allows us to overcome limits of planar structuring techniques.

To date, most ion-track applications are based on chemical etching, which dissolves the track material preferentially and creates fine channels of a few nanometers up to several micrometers in diameter. The superior properties of ion track membranes are related to the well-defined number and uniformity of diameter, length, and shape of the pores. Various examples will be presented such as perforated micromoulds, microfluidic systems with integrated nanoporous filter zones, and templates for the growth of nanowires. Polymer foils containing one single conical nanopore are suitable for biosensor applications and exhibit interesting ion-transport properties. Governed by the properties of the internal surface, synthetic nanopores function as a voltage gate, rectify ion currents, and show voltage-dependent fluctuations with kinetics similar to voltage-gated biological ion channels.

Invited Talk DS 24.2 Thu 10:00 H 2013

Low energy maskless implantation with high lateral resolution. — •Jan Meijer[1], Sebastien Pezzagna[1], Dirk Reuter[2], Ivo W. Rangelow[3], Hartmut Wiggers[4], Fedor Jelezko[5], Inam Mirza[5], Jörg Wrachtrup[5], Ferdinand Schmidt-Kaler[6], Wolfgang Schnitzer[6], and Kilian Singer[6] — [1]RUBION, Ruhr-Universität Bochum — [2]Angewandte Festkörperphysik, Ruhr-Universität Bochum — [3]Mikro- und Nanoelektronische Systeme, TU-Ilmenau — [4]Institut für Verbrennung und Gasdynamik, Universität Duisburg-Essen — [5]3. Physikalisches Institut, Universität Stuttgart — [6]Quanteninformationsverarbeitung, Universität Ulm

The fabrication of scalable quantum computers based on solid state materials requires tools to manipulate and implant single atoms, clusters or molecules with nm resolution or below.

The technical requirements to meet this challenge are enormous. In the first approach, we will present a technology able to implant ions through an AFM-tip with a small hole. This technique is already realized in Bochum. It allows a maskless implantation of small structures using different types of ions and energies between 0.5 - 5 keV. In the second step, this method will be combined with an ion trap as a single ion source. This method will be developed at the University of Ulm. Calculations show that this enhancement offers the implantation of countable ions with a lateral resolution below one nm. The paper will give an overview of the status of these methods as well as the first results to apply single ion implantation in the fabrication of NV centres in diamond as a solid state room temperature qubit.

Invited Talk DS 24.3 Thu 10:30 H 2013

Cluster ion-surface interactions: from meV to MeV energies — •Kai Nordlund, Kristoffer Meinander, Tommi T. Järvi, Jarkko Peltola, and Juha Samela — Accelerator Laboratory, University of Helsinki, Finland

The nature of cluster ion-surface interactions changes dramatically with the kinetic energy of the incoming cluster species. In this talk I will review some of our recent work on the nature of cluster-surface interactions spanning an energy range from a few meV/cluster to about 1 MeV/cluster and cluster sizes in the range of 10 - 1000 atoms/cluster.

In the energy range of a few meV/cluster ion, the kinetic energy of the incoming ion is insignificant compared to the energy gained when the surface potential energy at the cluster-surface interface is released and partly translated into kinetic energy. Even in this energy regime I will show that surprisingly drastic effects can occur. When the energy of the incoming cluster is raised to a few eV/atom, the kinetic energy of the incoming cluster starts to affect the deposition. It will cause the cluster to entirely reform on impact. When the energy is raised to the range of keV's/cluster, the clusters start to penetrate the sample, fairly similar to conventional ion implantation. However, in dense targets the cluster ions may stick close to each other long enough to cause a significant enhancement of the heat spike in the material. Finally, I will show that at kinetic energies around 1 MeV/cluster the cluster enhancement of the heat spike may lead to dramatic surface effects.

DS 25: Trends in Ion Beam Technology: From the Fundamentals to the Application

Time: Thursday 11:15–13:00 Location: H 2013

DS 25.1 Thu 11:15 H 2013

Nano-Structures made by Swift Heavy Ions — •Wolfgang Bolse[1], Hartmut Paulus[1], Thunu Bolse[2], and Lothar Bischof[3] — [1]Institut für Halbleiteroptik und funktionelle Grenzflächen, Universität Stuttgart — [2]Institut für physikalische Chemie, Universität Stuttgart — [3]Institut für Ionenstrahlphysik und Materialforschung, Forschungszentrum Rossendorf

Recently we have discovered that the irradiation of thin oxide films with swift heavy ions (SHI) at small incident angles results in an instability of the film against periodic cracking and subsequent reorganisation on a sub-micron level due to ion hammering. Varying the conditions during irradiation (ion species, rotating the target) we were able to generate a wide range of nano-structures and patterns, the most interesting of which was an array of NiO-nanopillars with a diameter of the order of 100 nm and a height of about 2000 nm. Unfortunately, the arrangement of these nanotowers was not regular. [1] To overcome this problem, we have prestructured the films by means of a focused ion beam with an array of perpendicular cuts of about 100 nm width and 1000 nm distance. In fact, the subsequent irradiation with SHI under grazing incidence and permanent target rotation results in an ordered array of the NiO nanotowers. To our surprise, the same treatment of TiO-films lead to an ordered pattern of holes.

[1] W. Bolse, T. Bolse, C. Dais, D. Etissa-Debissa, A. Elsanousi, A. Feyh, M. Kalafat, H. Paulus, Surf. Coat. Technol. 200 (2005) 1430

DS 25.2 Thu 11:30 H 2013

Experimental demonstration of a determinstic single ion source with an expected implantation resolution of a few nm — •Kilian Singer, W. Schnitzler, N. M. Linke, J. Eble, and F. Schmidt-Kaler — Universität Ulm, Institut für Quanteninformationsverarbeitung, Albert-Einstein-Allee 11, D-89069 Ulm

We have realized a universal deterministic single ion source on the basis of an ion trap applicable to a wide range of elements and molecules[1]. Initially, cold $^{40}Ca^{+}$ ion crystals are trapped within a segmented linear trap. Those ions are then deterministically extracted and shot into a detector at a distance of 25 cm from the trap. With single ions, more than 90% of these extractions were successful. The kinetic energy distribution of the ions amounts to less than 0.1%. We have also demonstrated the extraction of mixed crystals containing other dopant ions. For the implantation with nm precision, we plan to utilize an electrostatic Einzel-lens to further improve the spatial resolution of the extracted ions. These can then be used to generate color centers in diamond for optical detection or to implant P into Si. Both systems provide the foundation for the realization of a solid state quantum computer [2,3]. In addition, the electrical properties of semiconductor devices can be greatly enhanced by the deterministic implantation of single ions [4].

[1] J. Meijer et. al., Appl. Phys. **A 83**, 321 (2006).
[2] F. Jelezko et. al., Phys. Rev. Lett. **93**, 130501 (2004).
[3] B. E. Kane, Nature **393**, 133 (1998).
[4] T. Shinada et. al., Nature **437**, 1128 (2005).

DS 25.3 Thu 11:45 H 2013

Fabrication of novel pinholes for digital in-line X-ray holography by FIB and their application — •Ruth Barth[1], Todd Simpson[2], Silvia Mittler[2], Michael Grunze[1], and Axel Rosenhahn[1] — [1]Angewandte Physikalische Chemie, Universität Heidelberg — [2]Department of Physics and Astronomy, The University of Western Ontario, Canada

One way of adapting the classical Gabor geometry for in-line holography to photons instead of electrons includes a pinhole which provides a diverging photon beam and a detector to record the hologram. As the resolution is determined by the wavelength of the photons and the numerical aperture of the detection system, it is straightforward to increase the photon energy in order to enhance the performance of the technique. Vacuum-ultraviolet (VUV) synchrotron radiation has been successfully utilized for this purpose, and the implementation of digital Gabor microscopy with 14 nm radiation was proven. As the effective numerical aperture is limited by the size of the central Airy maximum, which is in turn inversely depending on the diameter of the pinhole, small apertures with sizes of the order of the wavelength are desired. We show the application of new pinholes produced by Focused Ion Beam milling through thin gold membranes. Due to the high aspect ratio of about 1:5 to 1:10 it is possible to obtain homogeneous illumination of the CCD chip by the central Airy maximum without direct beam contribution. With these new point sources for soft X-ray holography reconstructions with resolution of presently 400 nm are possible.

DS 25.4 Thu 12:00 H 2013

Optical anisotropy induced by oblique incidence ion bombardment of Ag(001) — •Herbert Wormeester, Frank Everts, and Bene Poelsema — Solid State Physics, MESA+ Institute for Nanotechnology,

Oblique incidence ion sputtering has become a widely used method for the creation of highly regular patterns of lines and dots. On a Ag(001) surface oblique incidence sputtering creates a ripple pattern that exhibits plasmonic features. The photon energy of the plasmonic feature depends on the ripple periodicity. The development of these anisotropic features was measured in-situ with the optical technique Reflection Anisotropy Spectroscopy (RAS) for 2 keV Ar ions with a flux of a few $\mu A/cm^2$ in a temperature range of 300 - 420K. With RAS, a periodicity of ripples above 200 nm is measured by a shift in photon energy of the plasmon resonance. Features with a smaller periodicity show a plasmon resonance around 3.65 eV. The Rayleigh-Rice description for scattering from a slightly rough surface enables to relate the measured plasmonic feature quantitatively to the ripple's rms, wavelength and wavelength distribution. Ripple patterns created with ions at 70° and 80° polar angles of incidence are compared. High resolution LEED measurements after sputtering are used to determine the facet angles of the created ripples.

DS 25.5 Thu 12:15 H 2013

Chemical epitaxy of quartz after alkali-ion implantation: luminescence and surface structure — Stanislawa Gasiorek[1], Juhani Keinonen[1,2], •Klaus-Peter Lieb[1], Pratap Sahoo[1], and Timo Savajaara[2] — [1]II. Physikalisches Institut, Universität Göttingen, D-37077 Göttingen — [2]Accelerator Laboratory, FI-00014 University of Helsinki

Doping of alpha-quartz by ion implantation leads to amorphization even at low fluences, but subsequent annealing in air or oxygen can restore the crystalline order (chemical epitaxy [1,2]). Here we report on measurements of Rutherford backscattering channeling (RBS-C) and cathodoluminescence (CL) spectra during chemical epitaxy of quartz irradiated with Na and Rb ions and annealed in 18O-gas. In particular, the variation of the damage profile and CL spectra (the latter taken at 10 K and 300 K) as functions of the Na-ion fluence will be discussed. The CL spectra at 10 K are dominated by a 2.90-eV band and differ greatly from the ones taken at 300 K. Conclusions concerning the underlying photoactive defect structures will be drawn. A spider-net type surface structure developing after Rb-ion irradiation was measured by means of atomic force microscopy.

[1] K. P. Lieb, in Encyclopedia of Nanoscience and Nanotechnology, vol. 3, H. S. Nalwa, Ed., Am. Scient. Publ. (2004) pp. 233-251.
[2] K. P. Lieb and J. Keinonen, Cont. Phys. 47 (2006) 305.

DS 25.6 Thu 12:30 H 2013

Ion beam induced effects at 15 K in z-cut$LiNbO_3$ — •Thomas Gischkat, Frank Schrempel, and Werner Wesch — Institut für Festkörperphysik,Friedrich-Schiller-Universität Jena

The primary effects of the damage formation in z-cut $LiNbO_3$ due to ion irradiation was investigated. Therefor the samples were irradiated stepwise and subsequently measured by means of Rutherford Backscattering Spectrometry (RBS) at 15 K without changing the temperature of the sample. The irradiation was done with 30 keV H-, 50 keV Li-, 160 keV O- and 350 keV Ar-ions at ion fluences between $5\times10^{11}\,cm^{-2}$ and $2\times10^{17}\,cm^{-2}$. The RBS measurements were performed with 1.4 MeV He-ions in steps of equal charges providing a series of subspectra. It was observed that the backscattering yield of the damaged region decreases with increasing number of subspectra indicating an annealing of defects as a consequence of the RBS measurement. The energy deposited into electronic processes by the analyzing He beam is mostly responsible for the observed defect annealing. The amount of annealing depends on the defect concentration

and the ion species. The undisturbed defect accumulation which will be observed without any effect of measurement was calculated for the different ion species by an analytical formula taking into account the He-beam induced annealing.

DS 25.7 Thu 12:45 H 2013

Channeling irradiation of $LiNbO_3$ — •Tobias Steinbach, Frank Schrempel, Thomas Gischkat, and Werner Wesch — Institut für Festkörperphysik,Friedrich-Schiller-Universität Jena

The influence of the crystal orientation on the damage formation of x- and z-cut $LiNbO_3$ single crystals irradiated with 550 and 750 keV Si-ions was investigated. The irradiation was carried out along the corresponding axial channel as well as at different tilt angles. The damage accumulation was investigated by means of Rutherford Backscattering Spectrometry (RBS/C). Because the channelled ions are prevented from close collisions with the target atoms, the projected range of the ions is increased and the number of defects created by channelled ions at a certain ion fluence is less compared to a random irradiation. As a consequence the damage distribution is shifted to larger depths if the irradiation is performed along low index crystallographic directions. Selected samples were etched at 40°C in a HF-solution of 3.7% and 40%, respectively. Compared to the random irradiation with 550 keV Si-ions, the etched depth increases by a factor of 1.4 and 1.2 if the irradiation is carried out along the x- and the z-axis, respectively. From the dependence of the shift of the damage peak on the tilt angle a critical angle to avoid channeling of about 1.35° was determined for 750 keV Si-ions.

DS 26: Birkholz

Time: Thursday 13:45–14:15 Location: H 2013

Invited Talk DS 26.1 Thu 13:45 H 2013

Profiling of Fibre Texture Gradients by Anomalous X-ray Diffraction — •M. Birkholz[1], N. Darowski[2], and I. Zizak[2] — [1]IHP, Im Technologiepark 25, 15236 Frankfurt (Oder) — [2]HMI & Bessy, Albert-Einstein-Str. 15, 12489 Berlin

Preferred crystallographic orientation or texture is a typically observed phenomenon in polycrystalline thin films. In numerous studies, moreover, the texture strength was found to increase with layer thickness. The effect is of practical relevance, since many applications require an intentionally perfect alignment of crystallites as, for instance, in piezoelectric layers of SAW devices. So far, sample series of increasing thickness had to be prepared with the texture strength to be determined for each sample to derive estimates of the texture gradient.

A recently introduced technique allows for the quantitative determination of a fibre texture gradient in a single thin film (M. Birkholz, JAC 40 (2007) 735). The method operates by varying the average information depth of the XRD measurement via changing the wavelength. If this variation encompasses an absorption edge of one of the elements present, sufficiently large variations of the x-ray attenuation arise that allow for texture profiling at different depths. As an example, a study of thin ZnO:Al films will be presented that were measured at Bessy II. These layers were found to exhibit large texture gradients with the highest value of 0.3 m.r.d./nm to occur in the initial growth phase, i.e. with a texture increase of 1 multiple of a random distribution every 3 nm. Summarizing, this new method enables the determination of texture gradients as required in many thin film projects.

DS 27: Trends in Ion Beam Technology: From the Fundamentals to the Application

Time: Thursday 14:30–16:00 Location: H 2013

Invited Talk DS 27.1 Thu 14:30 H 2013

Surface engineering with ion beams: from self-organzied nanostructures to ultra-smooth surfaces — •Frank Frost, Bashkim Ziberi, Axel Schindler, and Bernd Rauschenbach — Leibniz-Institut für Oberflächenmodifizierung e. V.

Low-energy ion beam sputtering, i. e. the removal of atoms from a surface due to the impact of energetic ions or atoms, is an inherent part of numerous surface processing techniques. Besides the actual removal of material, this surface erosion process often results in a pronounced alteration of the surface topography. Due to different roughening and smoothing mechanisms a multitude of topographies can result from surface erosion. Under certain conditions, sputtering results in the formation of well ordered patterns. This self-organized pattern formation is related to a surface instability between curvature dependent sputtering that roughens the surface and smoothing by different surface relaxation mechanisms. If the evolution of surface topography is dominated by relaxation mechanisms surface smoothing can occur.

In this presentation the current status of self-organized pattern formation and surface smoothing by low-energy ion beam erosion is summarized. In detail it will be shown that a multitude of patterns as well as ultra smooth surfaces can develop, particularly on Si surfaces. Additionally the most important experimental parameters that control these processes and theoretical approaches describing the surface topography evolution are discussed. Finally, examples are given for the application of low-energy ion beams as a novel approach for passive optical device engineering for many advanced optical applications.

Invited Talk DS 27.2 Thu 15:00 H 2013

Rare earth doping of GaN — •André Vantomme — Instituut voor Kern- en Stralingsfysica and INPAC, K.U.Leuven, Celestijnenlaan 200 D, B-3001 Leuven, Belgium

Group III-nitrides, e.g. GaN, are suitable hosts for incorporating rare earths (RE), potentially resulting in visible light emission at various wavelengths. Ion implantation is commonly employed for semiconductor doping, presenting several advantages over other techniques, such as in situ doping. However, implantation induces radiation damage to the lattice, which can have detrimental effects on the electrical and optical properties of the material. Further, the exact lattice site of the implanted ions has to be known, since it strongly influences the intensity and splitting of the optical transitions. We have studied the defect accumulation during RE (Er, Eu, Tm) implantation into GaN, as well as the lattice site of the implanted ions, varying a range of experimental parameters such as the implanted fluence, temperature, angle of the beam incidence, energy, annealing conditions The defect concentration and profile were assessed by channelling spectroscopy and high-resolution X-ray diffraction. By emission channelling, the lattice site of implanted radioactive ions was accurately determined, including the root mean square displacement from the ideal sites. From our study, we derived a general model correlating the induced defects, strain and the ion lattice sites, irrespective of the implantation parameters. Finally, these structural properties were linked to the optical and electrical characteristics of the nitride, investigated by photo- and cathodoluminescence and by deep level transient spectroscopy respectively.

Invited Talk DS 27.3 Thu 15:30 H 2013

Junction and Channel Engineering for Advanced Microprocessors — •Manfred Horstmann — AMD Saxony LLC & Co. KG, Wilschdorfer Landstraße 101, 01109 Dresden, Germany

An overview of state of the art Silicon on Insulator CMOS transistors used for 65 nm/45 nm volume manufacturing of multicore microprocessors will be given. AMDs unique technology and transistor progression model as well as the key challenges to increase the performance per watt of microprocessor products will be described. For advanced SOI transistors stress engineering has become a standard feature since the 90 nm technology node due to gate oxide scaling limitations [1]. Especially techniques which induce local strain such as compressive and tensile stressed over-layer films, embedded-SiGe, and stress memorization, are key to enhance transistor and product performance [2]. To reduce the lateral and vertical device dimensions advanced (Laser or

Flash) annealing in combination with low energy implants has been applied [3]. These anneal processes yield an improved dopant activation for active and gate regions resulting in lower source-drain resistance and gate depletion without any additional diffusion. Starting with the 45nm node, reducing parametric scattering for instance by improving tilt, twist, energy etc. control of implant steps are an emerging topic for performance optimization. A novel technique to statistically investigate parametric scattering, directly in the microprocessor chip, will be presented.

[1] M. Horstmann, et al., IEDM 2005, p. 243 [2] A. Wei et al., VLSI 2007 [3] Th.Feudel et al., RTP Conference, Kyoto, 2006

DS 28: Trends in Ion Beam Technology: From the Fundamentals to the Application

Time: Thursday 16:15–17:45 Location: H 2013

DS 28.1 Thu 16:15 H 2013

Epitaxial TiN film deposition at different substrate temperatures using hyperthermal titanium ions — •J. W. Gerlach, A. Wolfsteller, T. Höche, and B. Rauschenbach — Leibniz-Institut für Oberflächenmodifizierung e. V., Permoserstrasse 15, 04318 Leipzig

Conventional ion beam assisted deposition (IBAD) of binary nitrides, e.g. TiN, is usually done by evaporation of the metal component and simultaneous nitrogen ion irradiation of the growing film. In the literature, a lot of consequences of this ion irradiation during film growth are reported like densification, enlargement of the crystallite size, change of the preferred orientation, biaxial texturing of the films, and others. Contrary, in the present contribution the growth of thin TiN films by deposition of titanium ions, possessing hyperthermal energies of several ten eV, in a nitrogen ambient is investigated. These hyperthermal titanium ions were produced by a pulsed dc vacuum arc metal plasma source. The TiN films were deposited at substrate temperatures in the range from 700 °C down to room temperature on Al_2O_3(0001) and MgO(100) substrates. The surface structure of the films was monitored in situ by RHEED. The crystallographic structure and texture was investigated by XRD. High resolution TEM was used to examine the morphology and defect structure of the films. The results show that all the deposited TiN films are epitaxial, even at RT, indicating the beneficial effect of the hyperthermal energy of the particles involved in the deposition process. The influence of the hyperthermal titanium ion irradiation on the crystalline quality of the films is discussed.

DS 28.2 Thu 16:30 H 2013

Ion beam synthesis of Mn/Sb clusters in silicon — •Michael Steinert[1], Andreas Undisz[2], Markus Rettenmayr[2], and Werner Wesch[1] — [1]Institut für Festkörperphysik, Friedrich-Schiller-Universität Jena — [2]Institut für Materialwissenschaft und Werkstofftechnologie, Friedrich-Schiller-Universität Jena

Sequential ion implantation was used to incorporate Mn and Sb ions at high fluences of $1\times10^{16}\,at/cm^2$ and $2\times10^{16}\,at/cm^2$, respectively, into weak p-type Si (0 0 1). The implantation was performed at temperatures of 200 °C and 350 °C with energies of 180 keV (Mn) and 350 keV (Sb). Channeling-RBS measurements carried out before and after a subsequent thermal treatment via rapid thermal annealing (RTA) at temperatures from 950 °C to 1350 °C for 30 s indicate a strong temperature dependent redistribution of the implanted species during the annealing process governed by the radiation caused defects. An increase of the c-RBS backscattering yield of Sb in all annealed samples suggests the formation of Sb-based clusters. Additionally performed cross-sectional TEM analyses, including EDX measurements, clearly show the presence of hexagonal shaped elementary Sb precipitates as well as compound-clusters consisting of Mn and Sb, which are aligned to the crystal structure of the host silicon. High resolution TEM indicates different crystalline phases inside the observed particles, for the most part deviating in orientation and atomic plane distance from the Si-matrix.

DS 28.3 Thu 16:45 H 2013

Diffusion contrasts of Gold in Silicon induced by ion bombardment — Xiangzun Wang, •Moritz Trautvetter, Andreas Klimmer, and Paul Ziemann — Universität Ulm

As has been demonstrated previously, the diffusion of Au at 250°C is clearly enhanced in amorphous (a-)Si as compared to that in (001)-oriented Si wafers [1]. This effect can be exploited to 'write' diffusion contrast patterns by ion bombardment through a mask leading to the local formation of a-Si. In this way, after subsequent annealing at an optimized temperature, a selective diffusion of Au into the amorphized parts can be accomplished which then exhibit a drastically enhanced electrical conductivity. In the present contribution, the lateral selective diffusion of Au will be demonstrated starting from a Au-covered part of the Si wafer into uncovered but ion bombarded parts of Si. Such experiments allow determination of the electrical conductivity of the Au containing parts.

[1] J. Ehrhardt, A. Klimmer, J. Eisenmenger, Th. Müller, H.-G. Boyen, P. Ziemann:Influence of ion induced amorphicity on the diffusion of gold into silicon, J. Appl. Phys. 100, 063534 (2006)

DS 28.4 Thu 17:00 H 2013

cavity layer introduction in SIMOX technology — •Xin Ou, Reinhard Kögler, Arndt Mücklich, Wolfgang Skorupa, and Wolfhard Möller — Institute of Ion Beam Physics and Materials Research, Forschungszentrum Rossendorf, PO Box 51 01 19, 01314 Dresden, Germany

Silicon On Insulator (SOI) is the next generation of integrated circuit technology and Separation by Implantation Oxygen (SIMOX) is one of the mainstream processes for SOI wafer fabrication. The high-dose oxygen implantation in commercial SIMOX process is the main disadvantage considering the wafer cost and quality. In this case, defect engineering is performed in SIMOX process, by introducing a cavity layer as a Oxygen gettering layer using low dose He, H in combination to O implantation and Internal Thermal OXidaiton (ITOX). The cavity layer will narrow the oxygen profile, enhance the growth rate of SiO_2 precipitates, and produce the vacancy defects recombining with the Oxidation released interstitials and reducing the strain in top Si layer. In this project, the width of the cavity layer, cavity size and position distribution, the percentage of empty volume are investigated in order to optimize the Oxygen gettering ability of the cavity layers by Transmission Electron Microscopy (TEM), Auger Electron Spectroscopy (AES), Fourier Transformed Infrared (FTIR) and Scanning Spreading Resistance Microscopy (SSRM). The thermodynamics and kinetics of the SiO_2 precipitates formation and the interaction between the SiO_2 precipitation and defects introduced by Oxygen and extra implantation were studied.

DS 28.5 Thu 17:15 H 2013

Controlled self-organization due to sputtering on Si surfaces by lithographic pre-patterning — •Bashkim Ziberi, Theresa Lutz, Renate Fechner, Dietmar Hirsch, Klaus Zimmer, Frank Frost, and Bernd Rauschenbach — Leibniz-Institut für Oberflächenmodifizierung e. V.

Pattern formation on the surface of different materials due to low-energy ion beam erosion is a versatile tool for large scale nanostructuring. However, usually this self-organization process lacks long-range ordering and a positional control of the evolving structures. One possibility to influence the ordering and lateral positioning of structures is by using pre-patterned substrate. In this way due to spatial limitations and guided by the lateral ordering of the pre-patterned templates the evolving topography shows an improved ordering, a fabrication principle also known as guided self-organization. In this contribution results on the ripple and dot pattern formation on pre-patterned Si surfaces during low energy ($\leq$ 2000 eV) Kr^++ and Xe^+ ion beam erosion are presented. 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. Examples are: i) formation of curved ripples on the surface, ii) perfectly square ordered dots on exact positions on the surface; iii) enhanced ordering of ripples and the formation of ripples with different orientation depending on the local surface orientation. iv) continuous and controlled change in orientation of ripples independent of the ion beam direction.

DS 28.6 Thu 17:30 H 2013

SAXS studies of ion-beam induced nano-sized silver metal

clusters in glass — •Ivo Zizak[1,2], Heinz-Eberhard Mahnke[1,3], and Vasil Koteski[1,4] — [1]Hahn-Meitner-Institute Berlin GmbH, Berlin, Germany — [2]Berliner Elektronenspeicherring-Gesellschaft für Synchrotronstrahlung mbh, Berlin, Germany — [3]Freie Universität Berlin, Berlin, Germany — [4]Vinca Institute, Belgrade, Serbia

In soda lime glass metallic nano-clusters are produced by incorporating the metal ions via ion exchange processes and subsequent energy input for reducing the ions to metal. By irradiation with swift heavy ions the resultant nanometer sized Ag metal clusters were found to be arranged in chains parallel to the direction of the ion beam [1,2]. For a more detailed and more quantitative study of the arrangement, the shape of the clusters, and the formation process, we have started small angle x-ray scattering (SAXS) experiments at the 7-Tesla-multipole-wiggler beam line at BESSY. The first SAXS images confirm the diameter of the Ag- metal droplets observed in transmission electron microscopy images. In an in-situ experiment during annealing with increasing temperature from room temperature up to 340°C (at this temperature Ag was incorporated by ion exchange) two fractions of scattering centers, increasing with rising temperature, are observed, which are assigned to clusters arranging in chains and clusters homogeneously distributed over the sample volume.

[1] J.J. Penninkhof et al., Appl. Phys. Lett. 83 (2003) 4137
[2] H.-E. Mahnke et al., Nucl. Instr. and Meth. B 245 (2006) 222

DS 29: Nanoengineered Thin Films

Time: Thursday 18:00–19:30 Location: H 2013

DS 29.1 Thu 18:00 H 2013

Glancing angle deposited Si nanostructures on differently patterned substrates — •Christian Patzig[1], Bernd Rauschenbach[1], and Bodo Fuhrmann[2] — [1]Leibniz Institute of Surface Modification, Permoserstraße 15, 04318 Leipzig, Germany — [2]Martin-Luther-Universät Halle, Heinrich-Damerow-Straße 4, 06120 Halle, Germany

The glancing angle deposition (GLAD) process is a sophisticated vacuum deposition method that allows for the growth of arbitrarily shaped, 3D structures on the nm scale. When the substrate is tilted during deposition in a way that the incoming particle flux strikes it under an highly oblique angle β (typically $\beta > 80°$ as measured to the substrate normal), self-shadowing conditions on the substrate surface lead to the growth of non-closed films, that consist of needles which are slanted towards the incoming flux of sputtered particles. In addition with an appropriate substrate rotation mechanism, different structures such as zigzags, vertical posts, spirals or screws can be sculpted. Here, the growth of Si nanostructures on bare Si substrates as well as on differently patterned substrates (electron beam lithography pre-patterned, nano sphere lithography pre-patterned) will be shown, and the influence of the periodicity and form of the used pattern on the growth of the structures will be discussed.

DS 29.2 Thu 18:15 H 2013

Nano pinhole lithography for the fabrication of complex lateral structure arrays — •Nadine Geyer, Huang Cheng, Bodo Fuhrmann, Frank Syrowatka, and Hartmut S. Leipner — Interdisziplinäres Zentrum für Materialwissenschaften, Martin-Luther-Universität, 06099 Halle (Saale), Germany

This work demonstrates the function of nano pinhole lithography. In this novel technique the image written by an atom-emitting arbitrary shaped macro-sized evaporation source is projected to the nm scale using the principle of a pinhole camera. For this purpose, regular arrays of pinholes are fabricated by modification of hexagonally closed packed monolayers of monodisperse polystyrene spheres. Thermal treatment of the layers yields nearly circular shaped voids between these spheres having uniform diameter and distance to the target substrate. Imaging is realized in a high vacuum thermal evaporation system, where the substrate with the pinhole mask is placed opposite to atom-emitting objects, which were in our approach bend tungsten wires of different shapes and electroplated with nickel. By using polystyrene spheres of different radii, the projection scale could be varied. Scales up to 1:100 000 and images with minimum line widths of < 50 nm could be obtained.

DS 29.3 Thu 18:30 H 2013

Self-assembled Fe nanowires on (2x3)N-induced Cu(110) surface — •Xiaodong Ma[1], Dmitri Bazhanov[1], Fikret Yildiz[1], Marek Przybylski[1], Valeriy Stepanyuk[1], Toshihiko Yokoyama[2], and Jürgen Kirschner[1] — [1]Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, 06120 Halle, Germany — [2]Institute for Molecular Science, Okazaki, 444-8585 Aichi, Japan

Nanometer-scale structures are of a great interest due to their potential applications in electronics. They can be grown on reconstructed (110) surfaces. A single layer of a copper nitride template was prepared on a single-crystalline Cu(110) surface by bombardment of nitrogen at elevated temperature. Room temperature scanning tunneling microscopy (STM) images with atomic resolution have clearly revealed a surface reconstruction showing a regular (2x3) periodicity, which was also confirmed by the low energy electron diffraction (LEED) pattern. After depositing Fe by molecular beam epitaxy (MBE) on the (2x3)N/Cu(110) template Fe nanowires were formed. STM images of the nanowires show their orientation along the [1-10] direction with a uniform width of 1.08 nm (which corresponds to three atomic distances along the [100] direction) and of monolayer height. The minimum separation distance between the nanowires is found to be exactly twice the periodicity of the template along [100]. When the coverage increases to a value above 0.5 ML double layer nanowires start form. *Ab initio* calculations were performed in order to understand the template reconstruction and the principles of the nanowire growth behaviour.

DS 29.4 Thu 18:45 H 2013

Metal nanostructure matrices through laser-patterning of thin films using phase mask projection — •Marisa Mäder[1], Jürgen Gerlach[1], Thomas Höche[1], Michael Lorenz[2], Marius Grundmann[2], and Bernd Rauschenbach[1] — [1]Leibniz Institute of Surface Modification, Permoserstraße 15, 04318 Leipzig, Germany — [2]Universität Leipzig, Institut für Experimentelle Physik II, Abteilung Halbleiterphysik, Linnéstraße 5, 04103 Leipzig, Germany

Metallic nanostructures feature a wide range of possible applications. Especially within the area of nanowire growth, well ordered matrices of substrate-bound metallic structures are qualified as catalysts. Furthermore, applications as biosensors, for surface enhanced Raman effect-driven phenomena, and for optical data transfer are conceivable. This paper presents very well ordered metal nanostructure matrices that are made by an interference technique called diffraction mask projection laser ablation. A thin metal film (Au, Ni, Ti, and others) is illuminated by a laterally varying laser intensity pattern. The pattern is created by phase mask projection and four-beamlet interference of an Excimer laser (KrF, 248 nm, 30 ns). The pattern is demagnified to nanoscales by passing a Schwarzschild objective. The film is removed from the substrate at positions of high laser intensities. The remaining film material melts and forms structures of minimized surface energy at the positions of the heat sinks. It is shown that nanodots-matrices (Au, Ni) as well as nano-gratings (Ti) form under different conditions. Additional, results of 3D-nanostructure growth using templates prepared by this technique are presented.

DS 29.5 Thu 19:00 H 2013

Physico-chemical Properties of Metal-Polymer Nanocomposite Films near the Percolation Threshold — •Vladimir Zaporojtchenko, Haile Takele, Christian Hanisch, Amit Kulkarni, Thomas Strunskus, and Franz Faupel — Chair for Multicomponent Materials, Technical Faculty of the CAU Kiel, Kaiserstrasse 2, D-24143 Kiel, Germany

The present talk reviews properties of metal-polymer nanocomposite films (MPNF) with high volume fractions of metal nanoparticles close to the percolation threshold. In this regime, the DC electrical conductivity and the permittivity are extremely sensitive to the nanoparticle concentration and separation. The morphology of the nanocomposites (particle size and distribution) prepared by PVD methods depends on the properties of the selected polymer and metal as well as on the preparation parameters, i.e. deposition rate and substrate temperature. As a consequence, a percolation threshold in the conductivity

was observed at different critical metal concentrations ranging from 15 to 40 vol. %. It is demonstrated also that the optical, electrical and chemical properties may be varied widely close to percolation. Thus the index of refraction can be tuned over a wide range and surface plasmons, occurring for noble metals in the visible range, can be shifted to the infrared region. MPNF chemical sensors are based on the swelling of the polymer matix in the presence of organic vapors. Moreover, new polymer-metal composites with photochromic properties will be presented.

DS 29.6 Thu 19:15 H 2013

Electrical characterization of conducting ion tracks in insulating tetrahedral amorphous carbon — •Hans-Gregor Gehrke[1], Anne-Katrin Nix[1], Johann Krauser[2], Christina Trautmann[3], and Hans Hofsäss[1] — [1]II. Physikalisches Institut Göttingen, Germany — [2]Hochschule Harz, Wernigerode, Germany — [3]Gesellschaft für Schwerionenforschung, Darmstadt, Germany

We investigated the formation and the electrical characteristics of quasi one-dimensional conducting tracks in tetrahedral amorphous carbon (ta-C) produced by swift heavy ion irradiation. The ta-C films with thicknesses of about 100 nm were created with mass-separated ion beam deposition (MSIBD) on highly conducting silicon substrates with a deposition energy of 100 eV yielding into a sp^3 bond fraction of approximately 80%. The films were irradiated afterwards with 1 GeV ^{238}U ions with fluences between 10^8 and 10^{11} ions/cm^2. The high electronic energy loss of about 30 keV/nm of the swift heavy ions graphitizes the film locally along the ion trajectory. Thus, conducting nanowires embedded in an insulating matrix were achieved. The presence of the tracks could be confirmed with atomic force microscopy (AFM) using a conducting cantilever and applying a bias voltage. The conductance of the tracks is several orders of magnitude higher than that of the surrounding matrix. Temperature depended electrical characterization (300 K - 15 K) were performed on track ensembles with special focus on improving the contact pads.

DS 30: Layer Properties: Electrical, Optical and Mechanical Properties

Time: Thursday 9:30–11:00 Location: H 2032

DS 30.1 Thu 9:30 H 2032

Spectral ellipsometry of embedded VO_2 nanoclusters in SiO_2 during the semiconductor-metal transition — Helmut Karl, •Anne-Kathrin Jambreck, and Bernd Stritzker — Institut für Physik, Universität Augsburg, D-86135 Augsburg

Vanadium dioxide exhibits a semiconductor-metal transition at 68°C. We have synthesized VO_2 nanoclusters embedded in 200 nm thick thermally grown SiO_2 on 4-inch silicon wafers by ion implantation. The elements V and O were implanted with an energy of 100 keV and 36 keV respectively in order to place the maximum concentration to a depth of approximately 100 nm in the SiO_2 thin film. The fluences of V and O were varied between 10^{17} and $4x10^{16}$ $\frac{at.}{cm^2}$ in order to achieve different V to O ratios and concentrations by a combinatorial ion implantation technique. After the implantation process the formation of the VO_2 nanoclusters was obtained by an annealing step in a rapid thermal processor in flowing Ar at 1000°C for 10 min. The formation of VO_2 precipitates was verified by Raman spectroscopy and x-ray diffractometry. The temperature dependent optical properties of the thin films were analysed by ellipsometry in the spectral range of 320 to 1700 nm. It was found, that the hysteresis of the optical parameters during the semiconductor-metal transition like refraction index n and extinction coefficient k as a function of temperature is much larger than that observed for VO_2 single crystals and thin films.

DS 30.2 Thu 9:45 H 2032

Stress-engineering and optical properties of SiO_2 and TiO_2 thin films grown by dual ion beam deposition — •Carsten Bundesmann, Inga-Maria Eichentopf, Stephan Mändl, and Horst Neumann — Leibniz-Institut für Oberflächenmodifizierung e.V., Permoserstr. 15, 04318 Leipzig

Reduced stress in thin films is a key issue for advanced optical applications, for instance, micro-mirrors. We present results on the influence of additional ion bombardment during growth on the layer stress and optical properties of SiO_2 and TiO_2 thin films. The thin films are grown by reactive dual ion beam deposition [1]. One ion beam source (sputter source) is used to sputter a target. An additional ion source (assist source) is used to bombard the film during growth. Thereupon, a non-thermal energy contribution is introduced into the top few monolayers, which can be used to tailor thin film properties, for instance, the layer stress [2]. Hence, layer stress and optical properties are investigated depending on the parameters of the sputter and assist source. It is found that the layer stress can be reduced by additional ion bombardment. The most important parameter is the ion energy of the assist source, whereas ion species and ion current have only a minor effect. The refractive index of the thin films changes only slightly and no absorption is introduced upon ion bombardment, which makes these thin films promising candidates for optical applications.

[1] C. Bundesmann, I.-M. Eichentopf, S. Mändl, H. Neumann, in submission.

[2] C. A. Davis, Thin Solid Films 226, 30-34 (1993).

DS 30.3 Thu 10:00 H 2032

Charge transport in nanoparticulate Zinc Oxide layers — •Simon Bubel[1], Donna Nikolova[1], Koshi Okamura[1], Norman Mechau[1], Roland Schmechel[2], and Horst Hahn[1] — [1]Forschungszentrum Karlsruhe, Institute of Nanotechnology — [2]Universität Duisburg-Essen, Institute for Nano Structures and Technology

The electrical characteristics of thin layers of nanoparticulate zinc oxide (*NP*-ZnO) were investigated by four-point–, current-voltage measurements and transient current experiments. Layers have been spin-coated from dispersion of *NP*-ZnO in isopropanol (iPrOH). The current injection from thermal evaporated metal electrodes of gold and aluminium was found to be ohmic. Accordingly, the influence of electrodes to the considered electrical characteristics of the nanoparticulate thin film could be neglected which enabled the application of space-charge limited current models. Therefore the potential gradient in the sample has been calculated and fitted to experimental data. The electrical properties observed were found in close agreement with the theory of traps distributed in energy.

DS 30.4 Thu 10:15 H 2032

Simulations on Grazing-Incidence Reflectometry in the XUV for Thin Film Structures — •Matus Banyay and Larissa Juschkin — RWTH Aachen - Department of Optical System Technology

Grazing-incidence reflectometry using extreme-ultraviolet light (XUV) of 4-40 *nm* enables to characterize thin film structures on the nanometer scale. Composition, thickness and surface roughness of a deposited layer system can be determined indirectly from its reflectivity curve by non-linear regression techniques and the combined Nevot Croce[1]- and general transfer-matrix formalism[2] for X-ray reflectivity. Here the reflectivity can either be determined as a function of incident wavelength at a fixed grazing angle or vice versa. This way it is even possible to specify a root-mean-square (rms) surface roughness of hidden layer-interfaces in the depth of a stack. We present our simulations on thin-film structures and materials that are of importance in XUV applications, e.g. *Si*, SiO_2, *Zn*, *C*, *Mo*, *Ag*. Results show that the amount of noise in the reflectivity curve imposes a boundary on the fitting precision. First data from laboratory based XUV-reflectometers is used to determine different layer-structures. Simulations on more complex systems (>10 layers) are planned. The results will help to estimate the possibilities of our planned experimental setup (supported by BMWi-InnoNet) that will be presented at the end of the talk while the main focus lies on the simulations.

[1] L. Nevot, P. Croce, Rev. Phys. Appl. 15, 761 (1980); [2] A. Gibaud, S. Hazra, Curr Sci., 78, 12 (2000);

DS 30.5 Thu 10:30 H 2032

Co-deposition of energetic carbon and Copper ions: Self-organization of multilayers — •Hayo Zutz[1], Dominika Lyzwa[1], Inga Gerhards[1], Carsten Ronning[1], Michael Seibt[2], and Hans Hofsäss[1] — [1]II. Physikalisches Institut, Universität Göttingen, Friedich-Hund-Platz 1, 37077 Göttingen — [2]IV. Physikalisches Insti-

tut, Universität Göttingen, Friedich-Hund-Platz 1, 37077 Göttingen

Multilayers grown by simultaneously deposition of carbon and Fe, Au, Cu or Ni ions reveal a self-organization process with alternately metal-rich and metal-deficient layers. The periodicities of these layers are of the size of a few nanometers. The metal-rich layers consist of crystalline clusters in an amorphous carbon matrix, while the metal-deficient ones of amorphous carbon with homogeneous distributed metal atoms. The concentration vs. depth distributions of the metal atoms were analyzed by Rutherford backscattering spectroscopy (RBS) and energy dispersive X-ray (EDX) spectroscopy measurements, while the structure of the films was examined via cross-section transmission electron microscopy (TEM). The results are in agreement with a model of the multilayer formation based on an interplay of sputtering, surface segregation, ion induced diffusion, and the stability of small clusters against ion bombardment. The optical absorption of these films was analyzed in the UV-Vis range with respect to the Cu content and the cluster size determined by X-ray diffraction (XRD) analysis.

DS 30.6 Thu 10:45 H 2032

Determination of yield stress and elastic modulus under complete consideration of substrate influence demonstrated on a-C:H films — •Matthias Herrmann, Maksim Karniychuk, Siegfried Peter, and Frank Richter — Institute of Physics, Solid State Physics, Chemnitz University of Technology, Germany

Much attention has been given to the mechanical response of diamond-like carbon (DLC) coatings such as amorphous hydrogenated carbon (a-C:H) because of their widespread applications as protective films for magnetic storage disks, optical parts, MEMS applications, and so forth. However, to successfully integrate DLC films into three-dimensional structures, a deeper understanding of the mechanical response of the films becomes necessary which can no longer be carried out by standard hardness testing. This is mainly addressed to more complex stress states within the material. To overcome this, the determination of parameters for elastic deformation (i.e. elastic modulus and Poisson's ratio) and critical stress states for the onset of inelastic deformation is expected to be more feasible for mechanical performance qualification. In the present study, a-C:H coatings deposited by a capacitively coupled r.f. PECVD process have been investigated in order to determine the film modulus, yield stress and yield strain. Therefore instrumented indentation experiments with spherical tips for elastic deformation and standard tests with sharp tips have been performed. The latter one enables to derive the yield stress from hardness tests by applying Pharr's concept of the effective indenter. The mechanical film properties are discussed in terms of the ion energy per deposited C-atom.

DS 31: Application of Thin Films

Time: Thursday 11:15–12:30 Location: H 2032

DS 31.1 Thu 11:15 H 2032

Piezoelectric thin film devices for biochip applications — •Kerstin Wätje[1,2], Jens Ebbecke[1,2,3], and Achim Wixforth[1,2] — [1]Universität Augsburg, Lehrstuhl für Experimentalphysik I, 86159 Augsburg — [2]Center of Nano Science, Geschwister-Scholl-Platz 1, 80539 München — [3]School of Engineering and Physical Science, Heriot-Watt University, Edinburgh, EH14 4AS, United Kingdom

"Lab-on-a-chip-devices" are well suited for the analysis of least amounts of liquids. Therefore, such systems are emerging from prototype status and cost effective materials for mass production are sought. For handling and mixing components, surface acoustic waves generated by piezoelectric elements are meanwhile routinely employed; however, the LiNbO3 single crystals usually used in such units are a significant cost factor. As an alternative, zinc oxide layers deposited onto glass substrates hold the promise of cheaper production and easier integration into the assembly. In the present study, experiments regarding the deposition of such layers using different plasma processes are presented. Film synthesis was performed using rf magnetron sputtering, pulsed laser deposition and plasma based ion bombardment of Sol-Gel films on crystalline and amorphous substrates. The impacts of significant deposition parameters are discussed. At optimum deposition parameters, excellent columnar growth in the preferred c-axis orientation could be observed. The suitability of such films for the desired biochip application is substanciated through first mixing experiments using optically lithographed interdigital transducers (IDTs).

DS 31.2 Thu 11:30 H 2032

Combinatorial development of ternary and quaternary shape memory thin film systems — •Robert Zarnetta[1,2], Sigurd Thienhaus[1,2], Alan Savan[2], and Alfred Ludwig[1,2] — [1]Institut für Werkstoffe, Ruhr-Universität Bochum, Germany — [2]Forschungszentrum caesar, Bonn, Germany

Current development goals for shape memory alloys in the area of conventional alloys are to decrease the transformational hysteresis to values below 5 K as well as to increase transformation temperatures to values above 100°C. In order to reach theses goals, thin film combinatorial and high-throughput technologies were applied. Ternary and quaternary materials libraries (continuous composition spreads) were deposited by optimized magnetron sputter techniques. The high-throughput characterization was performed by automated EDX (composition), XRD (microstructure), as well as temperature-dependent resistivity measurements revealing the phase transformation properties of the thin films. Temperature-dependent stress measurements on micro-structured cantilever Si-wafers with integrated 4-point resistivity measurement on each cantilever in a temperature range from -100°C up to 600°C were applied to characterize the actuator behavior. Results are presented for ternary Ni-Ti-X (X = Cu, Pd, Hf, Ag, ...) and quaternary Ni-Ti-Cu-Pd systems. Next to extending the knowledge about transforming compositions in ternary systems, special compositions or compositional regions with optimized properties were found.

DS 31.3 Thu 11:45 H 2032

Design, Characterization and Applications of Broadband MoSi- Multilayer Mirrors for Attosecond XUV Pulses — •Michael Hofstetter[1], Andy Aquila[3], Eleftherios Gouliemakis[2], Martin Schultze[2], Matthias Uiberacker[1], Eric Gullikson[3], David Attwood[3], Ference Krausz[2], and Ulf Kleineberg[1] — [1]LMU Munich — [2]MPI for Quantum Optics — [3]CXRO Berkeley Lab

Multilayer(ML)-coated XUV mirrors in combination with ultrathin metal transmission filters are known to be very suitable for spectral filtering and guiding of single attosecond (asec) XUV pulses from the near-cutoff region of High Harmonic Generation (HHG) sources in rare gases. We report on the design of periodic and aperiodic, broadband (15 - 30 eV) Mo/Si ML centered at ≈ 85 eV, theoretically developed by a needle algorithm code (optilayer) for optimum pulse response. Recent results published have demonstrated the filtering of single 170 asec pulses, recorded in XUV pump/IR probe streaking experiments, using an additional 150 nm Zr filter.[1] Even shorter pulse durations towards the (sub) 100 asec range are expected. The ML stacks have been fabricated by advanced Dual Ion Beam Deposition (DIBD) controlled by in-situ ellipsometry and ex-situ characterized by synchrotron radiation measurements at the Advanced Light Source. Finally, the extension of asec ML mirror technology towards higher photon energies exceeding 100 eV using different materials (La and B_4C) will be discussed, which could enable new photoemission experiments on solid surfaces with sub 100 asec time resolution.

[1]New Journal of Physics 9 (2007) 243

DS 31.4 Thu 12:00 H 2032

The influence of dc sputtered ZnO:Al/a-Si:H/c-Si heterostructures — •René Köhler[1,2], Andreas Schöpke[2], Sviatoslav Shokhovets[1], Gerhard Gobsch[1], and Manfred Schmidt[2] — [1]Technische Universität Ilmenau, EXP I, Weimarer Straße 32, D-98693 Ilmenau, Germany — [2]Hahn-Meitner-Institut Berlin, Kekuléstraße 5, D-12489 Berlin, Germany

Transparent conductive oxides (TCO's) are an essential part of optoelectronic and photovoltaic devices. In ZnO:Al/a-Si/c-Si heterostructure solar cells, one cruicial point for the performance of the device are interface states at the a-Si/c-Si interface which may influence the band bending in c-Si at this interface. The aim of this work was to find out whether the ZnO:Al deposition by reactive dc magnetron sputtering

does affect the properties of the a-Si:H/c-Si interface. For this purpose, the large signal photovoltage method (SPV; laser pulse excitation 910 nm, 162 ns pulse length) was used to measure the band bending in c-Si before and after ZnO:Al deposition and after removing the ZnO:Al film by etching in HCl. So, from the variation in the SPV signal we can draw conclusions about the influence of the sputter deposition process on the properties of the a-Si/c-Si interface.

DS 31.5 Thu 12:15 H 2032

Application aspect of the silicon light emitters — •Charaf Cherkouk, Lars Rebohle, Slawek Prucnal, Wolfgang Skorupa, and Manfred Helm — Institute of Ion Beam Physics and Materials Research,Forschungszentrum Dresden-Rossendorf (FZD), POB 51 01 19 Dresden Germany

The immediate and accurate monitoring of chemical and biological substances is the key issue in environmental analysis for minimizing the health risk for citizens and their exposure to pollutants. Recently, considerable attention has been focused on endocrine-disrupting compounds EDCs, such as estrogens, which constitute a wide group of environmental pollutants, especially in drinking water. A new concept for measuring the concentration of such organic compounds by using Si-based integrated light sources for fluorescence analysis is presented. In that concept the analyte, estrogen in this example, is labelled with a Fluorescence marker with a large Stokes shift and is immobilized at the passivated surface of the light emitter by receptor molecules. This simple labelling opens a way to extremely small device dimensions and is of great interest for point-of-care measurements. The current system has been characterized by FTIR, Raman and electroluminescence measurements.

DS 32: Metal and Amorphous Layers

Time: Thursday 13:15–14:30 Location: H 2032

DS 32.1 Thu 13:15 H 2032

Electronic structure of ultrathin lead films — •Yvonne Käsler, Andreas Nuber, Frank Forster, and Friedrich Reinert — Universität Würzburg, Experimentelle Physik II, 97074 Würzburg

We have prepared ultrathin lead films on a $Si(111)-(7\times7)$ surface using a low temperature growth method, which is necessary to mitigate the problem of a large lattice mismatch and a different chemical bonding of the metal film and the semiconductor. Using high resolution photoelectron spectroscopy we focussed on the observation of quantum well states (QWS) of different film thicknesses. As the formation of QWSs greatly modulates the electronic structure near the Fermi level it has been speculated before that a lot of other properties are modulated as well. One of these is superconductivity. We measured the QWSs at different thicknesses and temperatures, determined the linewidths, and thus we were able to calculate electron-phonon coupling parameters and transition temperatures in dependence of the overlayer thickness. We were able to observe deviations from the bulk values of these parameters.

DS 32.2 Thu 13:30 H 2032

Infrared spectroscopic study of chromium film growth on single crystal diamond — •Robert Lovrincic and Annemarie Pucci — Kirchhoff-Institut für Physik der Universität Heidelberg

Detectors made of single crystal diamond are currently being developed for several tasks in particle physics experiments. One important step towards satisfying detector performance is the metallization. As chromium is a carbide forming metal and therefore shows good adhesion to the diamond surface, we studied the system Cr/C(100) by means of infrared spectroscopy under ultra high vacuum conditions. By analysing the obtained spectra with a Drude type dielectric function, we are able to distinguish between different phases in the film growth and to derive information about the electrical conductivity of the metal layer.

Supported by EC Integrated Infrastructure Initiative Hadron Physics, Project RII3-CT-2004-506078

DS 32.3 Thu 13:45 H 2032

Crystallization kinetics of phase change materials — •Michael Klein, Tobias Sontheimer, and Matthias Wuttig — I. Physikalisches Institut (1A), RWTH Aachen, 52056 Aachen, Germany

Phase change materials are fascinating materials. They can be rapidly switched between two metastable states, the amorphous and crystalline phase, which show pronounced contrast in their optical and electrical properties. They are already widely used as the active layer in rewritable optical media and are expected to be used in the upcoming phase change random access memory (PRAM).

Here we show measurements of the crystallization kinetics of chalcogenide materials that lead to a deeper understanding of these processes. This work focuses mainly on the Ge-Sb-Te system but also includes Ag-In-Te materials.

The crystallization behaviour of these materials was investigated with an ex-situ annealing method employing the precise oven of a differential scanning calorimeter and imaging techniques employing atomic force microscopy and optical microscopy.

DS 32.4 Thu 14:00 H 2032

The field dependence of ageing processes: Ion migration in amorphous aluminum and tantalum oxide films after potentiostatic formation — •Kevin Stella and Detlef Diesing — Fachbereich Chemie and Centre for Nanointegration (CeNIDE), Universität Duisburg-Essen, D-45117 Essen, Germany

Anodic oxidation of thin aluminum and tantalum films was performed in an electrochemical droplet cell. Thicknesses from 2 up to 8 nm were employed on 10 nm thick aluminum and tantalum films. Under Ultra High Vacuum conditions the conductivity of the remaining metal film is monitored as function of time. Equally prepared oxide films were accomplished in metal–insulator–metal capacitors, which were used to monitor the capacitance as a function of time. The combination of the two experimental setups shows clearly, that small losses in the capacitance of aluminum oxide capacitors are due to slight thickening of the oxide even under vacuum conditions. Up to one monolayer of the base aluminum electrode can be oxidized during $10^5 s$. Modelling in terms of migration of either oxygen anion interstitials or metal cation migration points preferably to the latter one. Tantalum oxide films of the same thickness show a much larger stability indicating either a lower content of mobile ions or a higher activation barrier for ionisation and migration.

DS 32.5 Thu 14:15 H 2032

Effect of the Si/SiO_2 interface on oxygen diffusion in SiO_2 — •Kirsten Sunder[1], Hartmut Bracht[1], Peter Fielitz[2], and Günter Borchardt[2] — [1]Institute of Materials Physics, University of Münster, Germany — [2]Institute of Metallurgy, Clausthal University of Technology, Germany

With down scaling of metal-oxide-semiconductor (MOS) transistors, the influence of the SiO_2/Si interface on Si and O diffusion in SiO_2 is becoming an important issue. The effect of defects generated at the interface on Si diffusion was investigated intensely by means of isotope heterostructures. It was concluded that SiO generated at the interface diffuses into the oxide and accelerates Si diffusion. The impact of these or different defects on O diffusion was not determined so far.

Performing diffusion experiments with $Si_3N_4/SiO_2/^{28}Si^{18}O_2/^{28}Si$ isotope heterostructures, that possess different thicknesses of the $^{28}Si^{18}O_2$ layer, the influence of the SiO_2/Si interface on O diffusion in SiO_2 was investigated.

DS 33: Surface Modification

Time: Thursday 14:45–15:30 Location: H 2032

DS 33.1 Thu 14:45 H 2032

Surface properties of medical CoCr alloys after plasma immersion ion implantation — •Johanna Lutz[1,2] and Stephan Mändl[2] — [1]Translationszentrum für regenerative Medizin, Universität Leipzig, Leipzig — [2]Leibniz-Institut für Oberflächenmodifizierung, Leipzig

Different medical CoCr alloys were treated with nitrogen plasma immersion ion implantation (PIII), an implantation method where the sample is immersed in a plasma and negative high voltage pulses are applied to it. This leads to the formation of surface layers with nitrogen contents up to 30 at.% and a thickness of more than 1 micrometer after 1 hour at 400 °C. This layer should exhibit an improved biocompatibility and mechanical surface properties.
Analysing the nitrogen diffusion data from SIMS measurements as well as the phase information data from XRD measurements and mechanical properties from nanoindentation and wear measurements, several conclusions can be drawn: the thermal activation energy for the nitrogen diffusion of about 0.5 eV indicates an interstitial diffusion path; at temperatures lower than 400 °C, a lattice expansion of the fcc base structure is observed, at higher temperature CrN precipitates are formed. At the same time, the hardness of the surface layers increases by a factor of 3 from 5 (untreated material) to 16 GPa with a corresponding increase in the wear resistance, nearly independent of the process temperature.

DS 33.2 Thu 15:00 H 2032

Field effect mobility and carrier concentration of graphitized polymer surfaces — •Y. Koval, I. Lazareva, and P. Müller — Institut für Physik der Kondensierten Materie, Universität Erlangen-Nürnberg, Erwin-Rommel Str. 1, 91058 Erlangen, Germany

Recently we have shown that surfaces of various polymers can be graphitized by low-energy ion irradiation [1]. Because of the low energy of ions, the thickness of the graphitized layers is less than 10 nm. By varying the irradiation conditions, the conductivity of the graphitized layers can be changed between 10^{-5} and 200 S/cm. This rather high conductivity makes graphitized layers interesting for several applications in microelectronics. We present our results of graphitized polyimide surfaces. We have found that the conductivity of low conducting samples can be described by variable range hopping, while highly conducting samples show a semi-metallic behavior. Field effect mobility and carrier concentration were determined for both low and highly conducting samples. It is worth to note that highly conducting surfaces show a field effect mobility as high as 5 cm^2/Vs. It was found that the rise of conductivity is caused by a simultaneous increase of the carrier concentration and the mobility of charge carriers. Moreover, a correlation between carrier concentration and mobility was found.

[1] I. Lazareva, Y. Koval, M. Alam, S. Strömsdörfer, P. Müller, Appl. Phys. Lett. 90, 262108 (2007)

DS 33.3 Thu 15:15 H 2032

Nano-patterning of diamond-like carbon by electron-assisted local oxidation in humid environment — •Thomas Mühl[1], Andreas Winkler[1], and Sverre Myhra[2] — [1]Leibniz-Institut für Festkörper- und Werkstoffforschung IFW Dresden, Helmholtzstr. 20, D-01069 Dresden — [2]Oxford University Begbroke Science Park, Department of Materials, University of Oxford, Oxford OX5 1PF, UK

Carbon-based materials such as diamond-like carbon (DLC) thin films and carbon nanotubes are attracting a great deal of attention due to their novel and versatile properties and likely applications. In particular, good chemical stability has been ascribed to these materials. Recently it has been shown that DLC can be patterned on the nm-scale by local electro-oxidation in a humid environment, where localization is defined by either "tunnel" current or spreading current in STM or AFM modes (Scanning Tunnelling and Atomic Force Microscopy), respectively. The process has now been extended to oxidative patterning of DLC films in an environmental SEM (Scanning Electron Microscope) in the presence of 10 to 100 Pa of water vapour.

Examples for nano-patterning of DLC thin films, both on substrates and self-supporting, will be presented. Preliminary data of the SEM-based process suggests that the volume removed by oxidation is linearly dependent on dose, approximately inversely proportional to the e-beam energy in the investigated energy range of 10 to 25 keV, while the dependence on partial pressure of water vapour has a minor effect.

DS 34: Hard and Superhard Coatings

Time: Thursday 15:45–16:45 Location: H 2032

DS 34.1 Thu 15:45 H 2032

Doping of high quality c-BN films epitaxially grown on top of diamond(001) — •Hong Yin[1], Xuyang Wang[1], Ivan Pongrac[1], Paul Ziemann[1], Fabian Renaux[2], Michel Hecq[2], and Carla Bittencourt[2] — [1]Institut für Festkörperphysik, Universität Ulm, 89069, Ulm, Germany — [2]University of Mons-Hainaut, B-7000 Mons, Belgium

Since it first synthesis in 1957 cubic Boron Nitride (c-BN) has attracted considerable interest due to its extreme physical and chemical properties. Besides as a superhard material second to diamond, it exhibits a wide band gap (6.4 eV) and high thermal conductivity making c-BN attractive as a high temperature electronic material. The recently achieved heteroepitaxial growth of c-BN films on top of diamond(001) [1] opened a promising window for e.g. c-BN/diamond pn-junctions. We will present results on the doping of high quality c-BN samples epitaxially grown onto diamond(001). XPS combined with ToF-SIMS results showed that metallic impurities within such epitaxial films are below several ppm leaving carbon and oxygen as the main impurities, which are homogeneously distributed inside the film. As a result, the nominally undoped c-BN films are p-type conducting as revealed by Hall effect. Si^+ was chosen to dope these epitaxial c-BN films by either in-situ adding Si^+ during film growth, or ex-situ doping by cold implantation and rapid thermal annealing (CIRA). In both cases, the electrical resistance of the samples is significantly decreased. Hall effect measurements indicate a related n-type conduction.

[1] X. W. Zhang et al., Nature Mater. **2** (2003) 312.

DS 34.2 Thu 16:00 H 2032

Abscheidung und Anwendungen von Kohlenstoffnitridschichten (CN_X) für Bauteile und Werkzeuge — •Ulrike Springborn[1], Katharina Köster[1], Mohammad Djahanbakhsh[2], Rolf Wäsche[2], Martin Keunecke[1] und Klaus Bewilogua[1] — [1]Fraunhofer Institut für Schicht- und Oberflächentechnik, Bienroder Weg 54 E, 38108 Braunschweig — [2]BAM Bundesanstalt für Materialforschung und -prüfung, 12200 Berlin

Bei den Versuchen zur Herstellung der superharten Phase des Kohlenstoffnitrids wurden interessante mechanische und tribologische Eigenschaften des Materials CN_X mit X zwischen 0 und 0,2 gefunden. Dazu gehören eine sehr geringe Oberflächenrauhigkeit, geringe Kontaktwinkel, hohe Elastizität und eine einstellbare Leitfähigkeit. Dünne CN_X-Schichten mit Schichtdicken von 10 nm und weniger werden in der Festplattenherstellung als Schutzschichten verwendet. Die Charakterisierung der tribologischen und mechanischen Eigenschaften dickerer CN_X-Schichten, zum Beispiel Härte, Verschleiß und Kontaktwinkel, soll eine mögliche Anwendung der CN_X-Schichten in der Bauteil- und Werkzeugbeschichtung untersuchen. Die CN_X-Schichten mit Schichtdicken bis zu mehreren Mikrometern werden hierfür mit dem in der Industrie weit verbreitetem Magnetronsputterverfahren unter variierenden Parametern hergestellt. Diese Parameter sind der Target-Substrat-Abstand, die Substrattemperatur und der Stickstofffluß. Ergebnisse aus den Untersuchungen zu Schichtzusammensetzung, Härte, Verschleiß, Reibungs- und Benetzungsverhalten werden dargestellt und diskutiert.

DS 34.3 Thu 16:15 H 2032

Scanning probe microscopy based characterization of reac-

tive sputter deposited coatings — •Thomas Klünsner[1], Gregor Hlawacek[1], Christian Teichert[1], Nazanin Fateh[2], Harald Köstenbauer[2], Gerardo Fontalvo[2], and Christian Mitterer[2] — [1]Institute of Physics, University of Leoben, Austria — [2]Dept. of Physical Metallurgy and Materials Testing, University of Leoben, Austria

Scanning probe microscopy, in particular atomic-force microscopy (AFM) with its derivatives, is suited for quantitative morphological characterization of thin solid films and the evaluation of their physical properties on the nanometer scale. Here, we applied atomic force microscopy in tapping mode to study the surface morphology of reactive magnetron sputtered V_2O_5 films on MgO(001) and TiN/Ag nanocomposite films as a function of substrate temperature or Ag content, respectively. Correlation function analysis was used to determine the rms roughness, the vertical correlation length, and the Hurst parameter. In addition, the AFM images revealed the three-dimensional shape of the plate-like crystallites formed in the polycrystalline phase above 80 °C. The results allow in conjunction with electron microscopy, x-ray diffraction and Raman spectroscopy to establish synthesis-structure relations of the film Finally, preliminary friction force microscopy measurements performed in contact mode will be presented to demonstrate the possibility to determine the friction coefficients of the coatings as a function of deposition conditions.

This work was supported by the Austrian NANO Initiative (Austrian Science Fund FWF) within the project "LowFrictionCoatings".

DS 34.4 Thu 16:30 H 2032

AlCrVN - Design of high-temperature low-friction hard coatings — •Robert Franz[1], Jörg Neidhardt[1], Markus Lechthaler[2], Peter Polcik[3], and Christian Mitterer[1] — [1]Christian Doppler Laboratory for Advanced Hard Coatings at the Department of Physical Metallurgy and Materials Testing, University of Leoben, Austria — [2]Oerlikon Balzers Coating AG, Balzers, Principality of Liechtenstein — [3]Plansee Lechbruck GmbH, Lechbruck, Germany

As environmental and economical considerations favour cutting with reduced coolants, controlling the friction becomes a major issue for the development of wear protective tool coatings. Common state-of-the-art coatings like AlCrN exhibit a relatively high friction especially at elevated temperatures, which leads to even higher thermal loads at the cutting edge and consequently to failure by thermal degradation. The incorporation of V into AlCrN results in a distinct reduction of the coefficient of friction at 700°C as the lubricious oxide V_2O_5 is formed. The new $Al_xCr_yV_zN$ coatings were synthesised by means of physical vapour deposition using an industrial-scale arc-evaporation system. The desired metastable face-centered cubic (fcc) structure was stabilised even at an Al concentration of x=0.7 by using higher energetic growth conditions. Due to this structural evolution hardness and residual stress values comparable to fcc-AlCrN were retained. Annealing experiments in ambient air at temperatures ranging from 550-700°C revealed the formation of a V-rich oxide scale due to the immiscibility of V_2O_5 with the other oxides formed (Al_2O_3 and Cr_2O_3).

DS 35: Nanostructured block copolymer films (SYSA 8)

Time: Thursday 17:00–18:30 Location: H 2032

Invited Talk DS 35.1 Thu 17:00 H 2032

Nanostructure and transport in regioregular polythiophenes and their block copolymers — Rui Zhang[1], Bo Li[1], Jessica R. Cooper[1], Mihaela Iovu[1], Genevevie Sauve[1], David N. Lambeth[1], Detlef-M. Smilgies[2], Richard D. McCullough[1], and •Tomasz Kowalewski[1] — [1]Department of Chemistry, Carnegie Mellon University , 4400 Fifth Avenue, Pittsburgh, PA 15213 — [2]Cornell University, Ithaca, NY, USA

This presentation will describe the results of combined atomic force microscopy (AFM) and grazing incidence small and wide angle x-ray scattering (GISAXS/GIWAXS) studies of narrow polydispersity regioregular poly(alkyltiophenes) (PATs) and their block copolymers. Well-defined PATs were shown to have a high tendency to form nanofibrillar structures with the nanofibril widths closely related to the contour lengths of polymer molecules. Moreover, carrier mobilities in field effect transistors fabricated from PATs exhibiting nanofibrillar morphologies exhibited exponential dependence on nanofibril width. The significance of this relationship as well as the morphology of block copolymers of PATs with immiscible segments and its impact on transport properties will be also discussed.

DS 35.2 Thu 17:30 H 2032

Morphological control in organic electronic devices using semiconductor block copolymers — •Sven Hüttner[1,2], Michael Sommer[2], Ullrich Steiner[1], and Mukundan Thelakkat[2] — [1]Cavendish Laboratory, University of Cambridge, UK — [2]Angewandte Funktionspolymere, Universität Bayreuth, Germany

Morphology plays a key role in organic electronic devices. In organic solar cells, for example, one important parameter is the creation of a large donor-acceptor interface for efficient charge separation while providing charge transport pathways to the respective electrodes at the same time. We address this issue by combining the concept of block copolymer self-assembly with functional polymers providing light absorption, hole transport and electron transport.

The presented block copolymer consists of an electron conducting block which is featured by a perylene bisimide derivative and a second block which is either featured by polystyrene or a hole conducting block such as polymerized triphenylamine derivatives. By applying different annealing methods, like the controlled exposure to solvent vapour, we can achieve highly ordered, self-assembled nanostructures of the two components with some tens of nanometers in scale. This is decisive for polymer photovoltaic devices.

Furthermore we have investigated these novel perylene bisimide based block copolymers and homopolymers in organic field effect transistors. The material shows excellent n-type properties with electron mobilities in the order of $10^3 \frac{cm^2}{Vs}$ and threshold voltages as low as 5V could be achieved.

DS 35.3 Thu 17:45 H 2032

Creating nano-structured films from self-encapsulated inorganic-organic hybrid materials — J. Perlich[1], M. Memesa[2], J.S. Gutmann[2], and •P. Müller-Buschbaum[1] — [1]TU München, Physik-Department LS E13, James-Franck-Str. 1, D-85748 Garching (Germany) — [2]MPI for Polymer Research, Ackermannweg 10, D-55128 Mainz (Germany)

Inorganic-organic hybrid materials are used in many technological areas. Nano-structured films of these materials are of special interest for photo-volatic applications. Based on a sol-gel process and an amphiphilic diblock copolymer matrix metal oxide nano-structures are created. These nano-structures are transferred into thin films and result in highly ordered hybrid films. Key parameters with respect to structural control are the type of diblock copolymer and the detailed preparation conditions. After thin film preparation a calcinations process is added. Moreover the impact of plasma etching is investigated. We focus on the example of poly(styrene)-b-poly(ethylenoxide), P(S-b-EO), for the preparation of the TiO2 nano-composite films, a system which exhibits optical properties for photo-volatic applications. Nano-structures on simple Si substrates are compared with structures obtained on ITO-covered glass surfaces. Experimentally the investigation is based on grazing incidence small angle x-ray scattering (GISAXS) in combination with scanning probe microscopy (SPM) and scanning electron microscopy (SEM). Each step of the complex preparation process is monitored with these techniques allowing for a high degree of control.

DS 35.4 Thu 18:00 H 2032

Thin films of diblock copolymers having one crystalline block — •Charles Darko[1], Ioan Botiz[2], Günter Reiter[2], Dag W. Breiby[3], Jens W. Andreasen[4], Detlef-M. Smilgies[5], Stephan V. Roth[6], and Christine M. Papadakis[1] — [1]Physikdepartment E13, TU München — [2]ICSI, CNRS, Mulhouse, France — [3]Norwegian University of Science and Technology, Trondheim, Norway — [4]Risø National Laboratory, Denmark — [5]Cornell University, Ithaca, USA — [6]HASYLAB at DESY, Hamburg

In thin films of symmetric poly(styrene-b-ethyleneoxide) (PS-b-PEO) diblock copolymers, the surface morphologies obtained are strongly

influenced by the internal structural rearrangement within the films which are associated with different mechanisms of crystal growth of PEO. With grazing incidence small and wide angle X-ray scattering, we obtained information about the mesoscopic structures as well as the crystallite orientations within the thin films. We observed lamellae parallel to the substrate in all films, but the internal structure and the degree of preferred orientation depends strongly on crystallization temperature: When crystallized at 25°C, the c-axis is oriented at approximately 35° with respect to the film normal with a broad distribution. At a crystallization temperature of 50°C, the c-axis becomes perfectly perpendicular to the substrate/film interface. The lamellar repeat distances increase with crystallization temperature. The information on the inner structures is compared to the surface textures measured by optical and atomic-force microscopy (AFM).

DS 35.5 Thu 18:15 H 2032

Temperature dependent X-ray diffraction studies of low and high molecular weight Poly(3-hexylthiophene) P3HT fractions — •Siddharth Joshi[1], Souren Grigorian[1], Ullrich Pietsch[1], Patrick Pingel[2], Achmad Zen[2], Michael Forster[3], and Ullrich Scherf[3] — [1]Festkörperphysik, Universität Siegen, Walter Flex strasse 3, D-57068, Siegen, Germany. — [2]Institut für Physik, Universität Potsdam, Am Neuen Palais 10, D-14469, Potsdam, Germany. — [3]Macromolecular Chemistry, Bergische Universität Wuppertal, Gauss-strasse 20, D-42119 Wuppertal, Germany.

GI-XRD in-plane and out-of-plane studies were performed in order to understand the crystallinity, the molecular orientation and the nanoscale morphology of a low-(LMW) and a high molecular weight (HMW) fractions of Poly(3-hexylthiophene) thin films along normal as well as parallel to substrate. Thickness dependence structural ordering has been also investigated for both fractions. At the same time we also correlated thickness dependence of structural ordering with corresponding electrical measurements for both fractions. LMW films are mainly amorphous and contain randomly oriented nano-crystallites with the best match for a monoclinic unit cell. For LMW material, the crystallites were preferentially orientation along the surface normal when the size of crystallites become in the order of film thickness i.e. ~ 20 nm. For HMW fraction we found an increase of lamellar ordering at about 60 K below the melting point of the material. Depending on substrate used (OTS, HMDS or SiO2) one can see a clear difference in the crystal orientation and packing at the interface region.

DS 36: Vibrational Spectroscopy of Nanolayers with Optical Probes

Time: Friday 10:15–12:00 Location: H 2013

Invited Talk DS 36.1 Fri 10:15 H 2013

Infrared ellipsometry on functional films at the solid-liquid-interface — •Karsten Hinrichs — ISAS - Institute for Analytical Sciences, Department Berlin, Albert-Einstein-Str. 9, 12489 Berlin, Germany

Organic/silicon hybrid systems are of high technological relevance for design of optical, electronic, biosensing and photovoltaic devices. Infrared spectroscopic ellipsometry (IRSE) was applied for in-situ monitoring of structural properties at the interface between silicon/film and liquid. Several examples with a few nm thick films at the solid-liquid interface will be discussed: 1) Etching process of anodic silicon oxide in diluted NH_4F solution; 2) The study of the switching behavior of stimuli-responsive mixed polymer brushes [1]; 3) The growth of electrochemically prepared organic films (e.g. polypyrrole, nitrobenzene).

[1] Y. Mikhaylova, L. Ionov, J. Rappich, M. Gensch, N. Esser, S. Minko, K.-J. Eichhorn, M. Stamm, K. Hinrichs, Analytical Chemistry 79 (2007) 7676.

Invited Talk DS 36.2 Fri 10:45 H 2013

Surface enhanced infrared spectroscopy — •Annemarie Pucci — Ruprecht-Karls-Universität Heidelberg, Kirchhoff-Institut für Physik, Im Neuenheimer Feld 227, 69120 Heidelberg

Surface enhanced infrared (IR) spectroscopy (SEIRS) is similar to surface enhanced Raman scattering (SERS) but its vibration signal enhancement is much less than that obtained with SERS; only up to three orders of magnitude in enhancement were achieved so far. The difference to SERS is based on the lower influence of local electromagnetic fields onto the signal enhancement. Electromagnetic field enhancement is the main enhancement effect in SEIRS and SERS and it is obtained with nano-structured metal films or with metal nanoparticles via plasmonic excitations of free electrons. Electromagnetic nearfield enhancement is strongest in nano-gaps and in proximity of sharp tips. Accordingly, metal particle systems close to percolation give a stronger effect in SEIRS of adsorbate vibrations than systems with lower or higher particle density. For single particles strong field enhancement in the IR can be obtained in case of a rod-like shape and a high aspect ratio. Such nanoantennas with length in the micrometer range behave similar to ideal antennas, which is qualitatively different to nanoparticles with resonances in the visible range. Exploiting the nearfield enhancement at the antenna resonance, SEIRS of molecules on the antenna allows extraordinary strong signal enhancement, which makes SEIRS to an interesting tool for medical and chemical sensing.

DS 36.3 Fri 11:15 H 2013

Infrared properties of ultra-thin metal films at and below the percolation threshold — •Bruno Gompf, Martin Alws, Martin Hövel, and Martin Dressel — 1.Physikalisches Institut, Universität Stuttgart

Whereas the optical properties of thicker metal films are well understood, little has been done at and below the percolation threshold especially in the infrared region. We have studied ultra-thin gold films on Si/SiO2 in the thickness range from 1 nm to 10 nm over a very broad frequency range between 500 cm^{-1} and 40.000 cm^{-1} with FTIR spectroscopy and spectroscopic ellipsometry. Thicker continuous films show a normal Drude behaviour, i.e. with increasing frequency the reflectivity decreases. Below the percolation threshold an anomaly occurs: in a certain spectral range the reflectivity becomes smaller than that of the bare substrate indicating an antireflection coating of nm thickness for infrared light. This anomaly can in principle be understood by the divergence of the dielectric function at the metal-to-insulator transition.

DS 36.4 Fri 11:30 H 2013

Resonance enhanced infrared spectroscopy using single gold nanowires — •Frank Neubrech[1], Shafqat Karim[2], Thomas Cornelius[2], Javier Aizpurua[3], and Annemarie Pucci[1] — [1]Kirchhoff-Institut für Physik, Universität Heidelberg, Germany — [2]Gesellschaft für Schwerionenforschung, Darmstadt, Germany — [3]Donostia International Physics Center, Donostia-San Sebastian, Spain

We performed enhanced vibrational spectroscopy of molecules adsorbed on individual gold nanowires using synchrotron light of the ANKA IR-beamline at the Forschungszentrum Karlsruhe. Spectroscopic IR-microscopy of nanowires with a length of a few nanometer and a diameter of about 100nm prepared by electrochemical deposition in polymeric etched ion track membranes reveals antenna like plasmon resonances in the relative transmittance spectra. For a demonstration of resonance enhanced spectroscopy we used an octadecanethiol (ODT) monolayer as adsorbate. Depending on the spectral position of the antenna-like resonance in relation to the absorption bands of ODT (2850cm^{-1} and 2919cm^{-1}) enhancement factors (enhanced absorption signal divided by not enhanced absorption signal) up to 300 000 can be achieved. Such high factors exceed the enhancement obtained by common surface enhanced infrared absorption techniques, e.g. rough films substrates, by at least 2 orders of magnitude.

DS 36.5 Fri 11:45 H 2013

IR spectroscopy for degradation studies of OLED emitter materials — •Martin Binder and Annemarie Pucci — Kirchhoff-Institut für Physik, Universität Heidelberg

We are doing Infrared Spectroscopy on new emitter materials for highly efficient organic light diodes (OLEDs). These materials are small organic molecules. In our experiments we can evaporate these molecules under UHV conditions on silicon and do IR spectroscopy *in situ*. Our special interest lies on the stability of the molecules, for example their behaviour under UV irradiation is investigated. Degradation of OLEDs is still one of the big challenges in that field and a consistent expla-

nation is missing. During irradiation with UV light the photoluminescence is observed and, as it is well known, the luminescence is decreasing. We found a relativly strong loss in luminescence and much smaller changes in the IR spectra of the layers.

DS 37: Vibrational Spectroscopy of Nanolayers with Optical Probes

Time: Friday 13:30–15:00 Location: H 2013

Invited Talk DS 37.1 Fri 13:30 H 2013

Ambient pressure spectroscopy of catalytically active nanostructures: Mind the gap! — •Günther Rupprechter — Institute of Materials Chemistry, Vienna University of Technology, Veterinärplatz 1, A-1210 Vienna, Austria

Recent advances in model catalysis and in spectroscopic methods that can operate at ambient pressure now enable us to investigate a catalyst in its active state, i.e. while it is functioning. Polarization-modulated infrared spectroscopy, sum frequency generation, and high-pressure photoelectron spectroscopy allow monitoring the transformation of catalysts from the "as-prepared" to the "active-state", which may involve pronounced changes in catalyst structure and composition. The ultimate goal is the characterization of the active sites. A number of case studies are presented for Pd-based catalysts (single crystals, thin films, oxide supported nanoparticles), that illustrate the dynamic behavior of catalytically active surfaces, with emphasis on the activity of Pd surface oxides for CO and methanol oxidation, and on surface carbonate formation. There is clearly a need to "mind the gap" between investigations under ultrahigh vacuum and those at ambient pressure, as well as to account for the inherent differences between supported nanoparticles and extended single crystal surfaces.

Invited Talk DS 37.2 Fri 14:00 H 2013

Near-field Infrared Nanoscopy and Nanospectroscopy — •Rainer Hillenbrand — Nano-Photonics Group, Max-Planck-Institut für Biochemie, 82152 Martinsried, Germany — CIC NanoGUNE Consolider, 20009 San Sebastian, Spain

Comprehensive material analysis in thin films and nanostructures requires ultrahigh-resolution microscopy providing high sensitivity to chemical composition, structural properties and local conductivity, among others. Conventional far-field optical spectroscopy offers such sensitivity, however, diffraction limits the spatial resolution to half the illumination wavelength. Near-field optical microscopy (SNOM) can overcome this drawback. Particularly its scattering-type version (s-SNOM) allows optical imaging with nanoscale spatial resolution, independent of the wavelength. In s-SNOM, the elastically scattered light from the laser illuminated tip of an atomic force microscope is recorded, simultaneously to topography.

Besides of a short introduction to the s-SNOM technique, I will demonstrate mid-infrared microscopy and spectroscopy at 20-30 nm spatial resolution. Applications such as material-specific imaging of thin films and single nanoparticles [1-3] and free carrier mapping in semiconductor devices [4] will be demonstrated.

[1] A. Cvitkovic, et al., Phys. Rev. Lett. 97, 060801 (2006)
[2] M. Brehm, et al., Nano Lett. 6, 1307 (2006).
[3] A. Cvitkovic, N. Ocelic, R. Hillenbrand, Nano Lett. 7, 3177 (2007)
[4] A. Huber, et al., Adv. Mater. 19, 2209 (2007)

DS 37.3 Fri 14:30 H 2013

Creation of highly confined longitudinal field modes for near-field excitation — •Johannes Stadler, Catrinel Stanciu, and Alfred Meixner — Institut of Physical Chemistry, University of Tuebingen, Germany

The focusing properties of a confocal microscope are not only crucial to enhance the resolution for confocal microscopy, but also define the confinement and thus the local field strength in the focus. In particular for tip-enhanced microscopy, having a tightly focused beam is extremely important in order to avoid having a strong background overlapping the tip-enhanced signals. More important, the polarization of light in the focal area should be longitudinal to efficiently excite the metallic tips. We show here that a parabolic mirror (PM) fulfils both requirements when used as a focusing element for tip-enhanced microscopy. When using a radially-polarized beam, the PM provides the smallest diffraction-limited spot that can be created using far-field optics. Due to the different focusing properties and apodization factors of the PM, the intensity in the longitudinal mode is remarkably higher than in comparable setups using aplanar lenses. The strong longitudinal fields and the local confinement offer perfect conditions for the excitation of a near-field tip with fewer background noise. First examples of near-field optical easurements with this new arrangement will be presented.

DS 37.4 Fri 14:45 H 2013

Near-field Raman Spectroscopy utilizing scattering by noble metal particles on SiGe samples — •Peter Hermann[1], Michael Hecker[2], Sebastian Pankalla[2], Jochen Rinderknecht[2], Phillip Olk[3], Marc Tobias Wenzel[3], René Kullock[3], Yvonne Ritz[2], Ehrenfried Zschech[2], Peter Kücher[1], and Lukas Eng[3] — [1]Fraunhofer CNT, 01099 Dresden, Germany — [2]AMD Saxony LLC & Co KG, Material Analysis Department, 01099 Dresden, Germany — [3]Institut für Angewandte Photophysik TU-Dresden, 01069 Dresden, Germany

Noble metal particles show very interesting and complex optical properties. One of the most striking phenomena encountered in these particles are electromagnetic resonances due to collective oscillations of the conduction band electrons. The excitation of plasmons leads to an increased light scattering and to an enhanced electromagnetic near-field. Due to the high optical resolution which can be reached by near-field measurements, tip enhanced Raman spectroscopy (TERS) therefore became an inevitable analytical method for probing stress related phenomena in the semiconductor industry. First TERS measurements on SiGe structures indicate a much better optical resolution as compared to far-field experiments. However, the full potential of this method is not exploited yet; for instance, the observed Raman signal enhancement stemming from SiGe as investigated here, contains a composition of several contributions, such as different far-field polarization modes, scattered light, as well as near-field contributions. Careful analysis of these contributions is inevitable for local mechanical stress analysis.

DS 38: Vibrational Spectroscopy of Nanolayers with Optical Probes

Time: Friday 15:15–16:45 Location: H 2013

Invited Talk DS 38.1 Fri 15:15 H 2013

Vibrational dynamics on the nanoscale — •Markus Raschke — Department of Chemistry, University of Washington, Seattle, USA

As the spatial dimensions of a medium shrink into the 1 to 100 nm range, concomitant changes in the time scales of the fundamental optical excitations can occur. Here, by combining scattering-type scanning near-field optical microscopy with ultrafast spectroscopy techniques provides simultaneous nanometer spatial and femtosecond temporal resolution. Using transient IR pulses we demonstrate spatio-temporal imaging of block-copolymer nanostructures. The vibrational free-induction decay probed in the optical near-field of the respective molecular subensembles carries information about spatial coherence and intermolecular coupling. In addition, the influence of the tip as an optical antenna on the radiative rates of the induced tip-sample polarization will be discussed.

Invited Talk DS 38.2 Fri 15:45 H 2013

UHV-based TERS on adsorbed molecules — •Bruno Pettinger and Jens Steidtner — Fritz-Haber-Institut der MPG, Faradayweg 4-6, D-14195 Berlin

In recent years tip-enhanced Raman spectroscopy (TERS) has proven to be a feasible tool for the local investigation of surfaces on a nanometer scale, in some cases with single molecule sensitivity [1]. So far, TERS experiments were performed in the gas phase and under atmospheric pressure, which entails some disadvantages as e.g. the possible contamination of the tip and the sample. Here we present a novel microscope based on a high-numerical parabolic mirror for focusing the laser to a minimum size spot and collecting the scattered light. The SPM and the essential optical components are combined on a rigid platform, which is mounted in an UHV system. Optical fibers connect this setup with remote laser and spectrograph. The focusing of the laser onto the tip apex and maximizing the scattered intensity is achieved by a five-axis alignment of the parabolic mirror by piezomotors. For dye adsorbates on smooth Au(111) samples, the approach of a STM tip boosts the Raman scattering signal from a small region with a diameter of only a few nanometers to a 4000-fold level, which means an underlying enhancement of TERS of 10^6 - 10^7. This huge enhancement causes in UHV only a minor photodecomposition, much in contrast to comparable experiments in air, and thus allows to move toward single molecule spectroscopy and microscopy. Preliminary results on this topic will be presented.

1. K.F. Domke et al., J. Am. Chem. Soc. 128, 14721 (2006).

Invited Talk DS 38.3 Fri 16:15 H 2013

Tip enhanced Raman scattering on biological samples — •Volker Deckert — ISAS - Institute for Analytical Sciences, Dortmund, Germany

Recently optical techniques that reveal lateral resolution well beyond the diffraction limit became more and more accessible. In particular the combination of near-field optics and Fluorescence spectroscopy proved to be very successful. Since Raman spectroscopy is a comparable insensitive spectroscopic technique progress here was much slower. Just with the combination of field-enhancing techniques, near-field optical techniques could be combined with Raman methods. Especially Tip-Enhanced Raman Scattering (TERS) is a technique that uniquely combines the best of he two worlds. Her applications on biological samples ranging from single cells, single virus particles, to single molecules will be shown. Thus demonstrating the capabilities of TERS. Specifically TERS experiments on a single RNA strand will be discussed and the issue of direct label free sequencing of DNA will be addressed.

DS 39: Magnetism in Thin Films: Interaction Phenomena and Heterostructures

Time: Friday 10:15–12:00 Location: H 2032

Invited Talk DS 39.1 Fri 10:15 H 2032

Vortex Manipulation in Superconductor/Ferromagnet Hybrid Nanosystems(*) — •Victor Moshchalkov — INPAC-K.U.Leuven, Belgium

Artificial hybrid superconductor-ferromagnet (S/F) systems have been used to reveal the interplay between competing superconducting and magnetic order parameters, and to verify the existence of new physical phenomena, including the domain-wall superconductivity (DWS) and the reversed domain superconductivity (RDS)(Nature Materials 3, 793 (2004), Phys. Rev. Lett. 95, 227003 (2005), Phys. Rev. Lett. 95, 237003 (2005), Appl. Phys. Lett. 90, 182501 (2007)). Low-temperature scanning laser microscopy (LTSLM) together with transport measurements were carried out on Nb/$PbFe_{12}O_{19}$ hybrids in order to reveal local variations of superconductivity induced by the magnetic field template produced by the ferromagnetic substrate. Comparative analysis of the LTSLM and the MFM images has convincingly demonstrated the presence of the RDS (Phys. Rev. Lett. 96, 247003 (2006)). Periodic arrays of magnetic dots were used to investigate tunable field-induced superconductivity caused by the local field compensation with the stray fields of the magnetic dots with a variable magnetization. Critical currents and nucleation of superconductivity were controlled by using different cycles to magnetize the dots (Phys. Rev. B, 74, 220509 (2006)).

(*) In collaboration with W. Gillijns, J. Fritzsche, N. Schildermans, Q.H. Chen, K. De Keyser, A. Silhanek, J. Van de Vondel, A. Aladyshkin, K. Vervaeke, C.C. de Souza Silva, C. Carballeira, Z.R. Yang, V. Metlushko, D. Koelle, H.Eitel,R.Kleiner, R.Szymczak

Invited Talk DS 39.2 Fri 10:45 H 2032

Investigating the interaction between single-crystalline antiferromagnetic films and ferromagnets — •Wolfgang Kuch — Freie Universität Berlin, Institut für Experimentalphysik, Arnimallee 14, 14195 Berlin

The lack of detailed understanding of the coupling between an antiferromagnetic (AF) and a ferromagnetic film (FM) is in part due to the incomplete characterization of the interface in the sputtered polycrystalline samples that are typically used. Investigations of the AF/FM interface coupling at well-characterized single-crystalline interfaces can help to tackle this issue. I will present combined magneto-optical Kerr effect (MOKE) and layer-resolved magnetic imaging studies using x-ray magnetic circular dichroism (XMCD) and a photoelectron emission microscope (PEEM) for the investigation of single-crystalline systems. I will focus on Fe in contact to the oxidic antiferromagnet CoO, grown epitaxially on Ag(001), and on metallic systems containing FeMn as antiferromagnet, deposited on Cu(001). The pronounced layer-by-layer growth of the latter provides the opportunity to controllably tune the interface roughness on the atomic scale. Interestingly, the antiferromagnetic ordering temperature of the FeMn layer depends strongly on the magnetization direction of the adjacent FM layer, providing clear evidence for a magnetic proximity effect in which the FM layer substantially influences the ordering temperature of the AF layer.

Results were obtained in collaboration with F. Offi, L. I. Chelaru, M. Kotsugi, J. Wang, J. Kirschner, R. M. Abrudan, J. Miguel, K. Lenz, and S. Zander.

DS 39.3 Fri 11:15 H 2032

FeZr-based multilayers – a frustrated XY system? — •Andreas Liebig[1], Panagiotis Korelis[1], Gabriella Andersson[1], Björgvin Hjörvarsson[1], Hans Lidbaum[2], and Klaus Leifer[2] — [1]Dep. of Physics, Uppsala University, Uppsala, Sweden — [2]Dep. of Engineering Sciences, Uppsala University, Uppsala, Sweden

Anisotropy and frustration terms can lead to a reentrant spin-glass state at low temperatures in the amorphous ferromagnet $Fe_{90}Zr_{10}$.

Here, we present a study of $Fe_{90}Zr_{10}/Al_{70}Zr_{30}$ amorphous multilayers, using MOKE and a SQUID magnetometry. The structural quality was verified using X-ray reflectivity as well as HR-TEM and the chemical composition was determined by RBS.

Interlayer exchange coupling across the amorphous $Al_{70}Zr_{30}$ layer is weak and the ordering temperature is therefore almost exclusively dominated by the thickness of the $Fe_{90}Zr_{10}$ layers. Multilayers with $Fe_{90}Zr_{10}$ layers in the nm range are found to have extraordinarily low remnant and coercive fields – in fact, so low that the definition of a magnetic transition temperature becomes difficult. The magnetization of the layers collapses, with exceedingly high susceptibility above the apparent ordering temperature.

A conceptual model of the transition will be given, involving the competition between the local anisotropy and the exchange coupling. The results can have far reaching consequences for the understanding of the interplay between finiteness and ordering. For example, the use of nearest neighbour interaction is found to be insufficient for describing the observations.

DS 39.4 Fri 11:30 H 2032

Highly ordered spin-state in an epitaxial spin-valve — •Frank Brüssing, Boris Toperverg, Hartmut Zabel, and Katharina Theis-Bröhl — Department of Physics 4, Ruhr-University Bochum, D-44780 Bochum, Germany

Several periods of Fe and Co films separated by Cr layers were grown on MgO (001) by molecular beam epitaxy to form an epitaxial spin valve superlattice. We adjusted the film thicknesses of Fe and Co to have similar magnetic moments in the both magnetic layers. In order to get a proper spin-valve behavior we have chosen a Cr spacer thickness which provides a week antiferromagnetic coupling. The quality of the layering and the epitaxial relationship were verified via x-ray methods. For investigating of the arrangement of the magnetic moments in the different magnetic layers we performed polarized neutron reflectometry studies in the as-grown state and with an applied magnetic field. Ferromagnetic and antiferromagnetic alignment between neigh-

boring Co and Fe layers can be recognized via intensity variations on the nuclear [Co/Cr/Fe/Cr] superlattice peaks which are different for odd and even orders. Interestingly, additional half-order peaks appear in the asgrown state indicating a new magnetic state. In this state an antiferromagnetic alignment between complete neighboring [Co/Cr/Fe/Cr] unit cells occurs suggesting a highly-ordered demagnetized state induced by dipolar interaction during growth. Applying a magnetic field destroys this state which also can not be recoverd during field reversal. This project was supported by the DFG via SFB491.

DS 39.5 Fri 11:45 H 2032

Structural characterization and magnetization profile of CoFeB/MgO multilayers for Magnetic Tunnel Junctions — •Miriana Vadalà[1], Kirill Zhernenkov[1], Max Wolff[1], Oleg Petracic[1], Kurt Westerholt[1], Boris P. Toperverg[1], Hartmut Zabel[1], Piotr Wisniowski[2], and Susana Cardoso[2] — [1]Experimentalphysik/Festkörperphysik, Ruhr-Universität Bochum, Germany — [2]INESC, Lisbon, Portugal

We present structural and magnetic results from the characterization of CoFeB/MgO multilayers sputtered at different deposition pressures on Si/SiO_2 substrates. From X-ray scans we obtain the layer thicknesses and the interface roughnesses. Magnetic measurements show different results depending on the growth conditions. For all samples the magnetic anisotropy is negligible as intended by the growth of amorphous CoFeB layers. For smooth layers (lower Ar pressure) one finds a step-like hysteresis curve, whereas the curves are strongly rounded for the rougher system (higher Ar pressure). This could hint to a more decoupled vs. a stronger coupled remagnetization behavior, respectively. To shed more light on the behaviour of the alloy at the interface to the MgO layer, we have taken polarized neutron reflectivity data [1]. Similar to the $FeCo/Al_2O_3$ system [2] we observe for the multilayer with rough interfaces a loss of a ferromagnetic correlation at remanence, indicating that each CoFeB layer forms an uncorrelated domain structure. Financial support EU-RTN ULTRASMOOTH, SFB 491 and BMBF 03ZA6BC1 are acknowledged.

[1] M. Wolff, et al. Thin Solid Films 515, 5712 (2007)
[2] S. Bedanta, et al , PRB 74, 054426 (2006).

DS 40: Magnetism in Thin Films: Interaction Phenomena and Heterostructures

Time: Friday 12:15–14:15 Location: H 2032

Invited Talk DS 40.1 Fri 12:15 H 2032

Influence of antiferromagnetic layers on the magnetization dynamics of exchange coupled thin films — •Jeffrey McCord — Institute for Metallic Materials, IFW Dresden, Germany

The strength of unidirectional and uniaxial anisotropy fields together with the effective damping parameter in different types of polycrystalline ferromagnet/antiferromagnet (F/AF; AF:NiO, IrMn) systems is investigated as a function of AF thickness and thermal history. It is shown that, independent of the occurrence of exchange bias, higher order exchange anisotropy terms can be induced. These findings are also compared to complementary magnetic domain studies.The role of the formation of an interfacial layer on coupling, anisotropy, and magnetic damping is discussed. The data implies that the spin structure inside the antiferromagnetic layer is responsible for exchange bias and the dominating contribution to coercivity, the interfacial structure for the overall coupling. The chemical F/AF boundary structure and the thermomagnetic history is relevant and can be used to tailor precessional frequency and magnetic damping of ferromagnetic layers over a wide range.

DS 40.2 Fri 12:45 H 2032

Epitaxial $SmCo_5$/Fe/$SmCo_5$ trilayers - a model system for exchange spring media — •Volker Neu, Katrin Häfner, and Ludwig Schultz — IFW Dresden, P.O. Box 270116, 01171 Dresden, Germany

Exchange coupled hard / soft magnetic nanocomposites have recently found a renewed interest in data storage application as exchange spring media, also named exchange coupled composite (ECC). Developed formerly to improve the energy density of a hard magnetic material by an intimate, direct exchange coupling to a soft magnetic phase with high saturation polarization, as exchange spring media, the soft magnetic phase initiates the switching at moderate fields and thus enables the writability, whereas the high anisotropy of the hard phase guaranties the desired thermal stability in zero field [1]. Epitaxial $SmCo_5$/Fe bilayers and $SmCo_5$/Fe/$SmCo_5$ trilayers with tunable switching behaviour [2] constitute a well defined model system for studying of the above mentioned coupling phenomena. We present time dependent magnetization relaxation data measured at different reversal fields, which allow to compare thermal stability and switching fields for single hard layers and bilayers and trilayers with varying thickness of the soft layer.

[1] Suess et al., Appl. Phys. Lett. 87, 012504 (2005). [2] Neu et al., J. Phys. D : Appl. Phys. 39 5116 (2006).

DS 40.3 Fri 13:00 H 2032

Magnetization reversal in laser-interference patterned Co/Pd multilayer films studied by full-field Kerr microscopy — •Min-Sang Lee[1], Jie Li[1], Björn Redeker[1], Philipp Leufke[2,3], Stephen Riedel[2], Paul Leiderer[2], Johannes Boneberg[2], Manfred Albrecht[2], and Thomas Eimüller[1] — [1]Junior Research Group Magnetic Microscopy, Ruhr-University Bochum, D-44780 Bochum — [2]University of Konstanz, Department of Physics, D-78457 Konstanz, Germany — [3]Forschungszentrum Karlsruhe, Institut für Nanotechnologie, 76021 Karlsruhe, Germany

We investigate magnetization reversal processes in Co/Pd multilayer systems with strong perpendicular magnetic anisotropy which have been structured using direct laser interference patterning technique into a variety of shapes, e.g., stripes, squares, and asterisk-shaped dots. The intense laser irradiation at interference maxima causes chemical intermixing at the Co/Pd interfaces leading to the modification of magnetic properties such as the creation of pinning centres and the reduction in the strength of magnetic anisotropy. Due to this effect, different types of magnetization reversal process were observed in different sample area depending on the laser intensity at which the area was irradiated. The observation was done at our new laser Kerr microscopy setup, where a CCD camera with max. 30 fps was used for fast image acquistion. It enabled us to record motion pictures of magnetization reversals, which will be presented in this contribution. The financial support for this work has been provided by the DFG through SFB 491, SFB 513, and Emmy Noether Programme.

Invited Talk DS 40.4 Fri 13:15 H 2032

Ion Beam Induced Magnetic Nanostructures — •Peter Varga — Inst.f.Allgemeine Physik, TU Wien, Austria

For iron films with 5 to 10 layers epitaxially grown on Cu(100) stabilization of the face-centered cubic (fcc) γ-phase (which is non magnetic,) can be obtained above room temperature. This is in contrast to bulk iron for which the fcc phase is stable only above 1184 K, whereas below this temperature the body-centered cubic (bcc) α-phase (which is ferromagnetic) is thermodynamically stable. Films with more than 10 layers will exhibit a spontaneous structural transition to the bcc structure with in palne magnetization whereas below 5 layers a strained bcc structure shows an out of plane magnetic moment at room temperature[1]. We have shown by STM (Scanning tunneling microscopy) with atomic resolution and LEED (Low Energy Electron Diffraction) that this 5-10 ML thick fcc Fe films undergo a transition from fcc to bcc by ion beam irradiation. Since iron is ferromagnetic only if it is bcc or at least strained bcc but never if it is fcc[1] this gives the possibility to transform a nonmagnetic film into a ferromagnetic one directly by ion bombardment and especially to form magnetic nanostructures with a size determined by the diameter of the used ion beam only [2].

[1] A. Biedermann et al. Phys. Rev. Lett. 86 (2001), pp. 464*467 and 87 (2001) 86103 [2] W.Rupp, B.Kamenik, R.Ritter, A.Biedermann, Ch.Klein, E.Platzgummer, M.Schmid, and P.Varga, to be published

DS 40.5 Fri 13:45 H 2032

Magnetic texturing of ferromagnetic films by sputtering induced ripple formation — •Hans Hofsäss[1], Kun Zhang[1], Michael Uhrmacher[1], and Johann Krauser[2] — [1]II. Physikalisches Institut, Universität Göttingen, 37077 Göttingen — [2]Fachbereich Au-

tomatisierung und Informatik, Hochschule Harz, 38855 Werningerode

Ripple patterns created by sputter erosion of iron thin films induce a correlated magnetic texture of the surface near region. We investigated the magnetic anisotropy as a function of film thickness and determined the thickness of the magnetically anisotropic layer as well as the magnitude of the magnetic anisotropy using MOKE and RBS measurements. Ripple patterns were created by sputter erosion with 5 keV Xe ions at 80° incidence with respect to the surface normal. For ion-fluences above 1x10^{16} cm^{-2} ripples with wavelengths of 30 nm - 80 nm oriented parallel to the ion beam direction are observed. MOKE measurements reveal a uniaxial magnetic anisotropy of the surface region of the films with orientation parallel to the ripple orientation. The magnetic texture is confined to a 12+/-3 nm thick layer, in accordance with the average grain size. The magnetic anisotropy within this layer varies from 25% for thick films towards 100% for films with less than 30 nm thickness. The magnitude of the anisotropy is determined by the shape anisotropy of the rippled surface as well as the interface roughness. We have demonstrated that sputter erosion yields highly anisotropic magnetic thin films and can be used to fabricate nanorods and nanowires with pronounced uniaxial magnetic anisotropy.

DS 40.6 Fri 14:00 H 2032

Magnetism of the Heusler compound $Co_2Cr_{0.6}Fe_{0.4}Al$ at interfaces with Cr and AlO_x — •Martin Jourdan[1], Elena Arbelo-Jorge[1], Christian Herbort[1], Timothy Charlton[2], and Sean Langridge[2] — [1]Institut für Physik, Johannes Gutenberg Universität Mainz, 55099 Mainz, Germany — [2]ISIS facility, Rutherford Appleton Laboratory, Oxfordshire OX11 0QX, UK

$Co_2Cr_{0.6}Fe_{0.4}Al$ (CCFA) belongs to the Heusler compounds for which a huge spin polarization is theoretically predicted. However, for spintronics applications the electronic properties at the interface with insulating barriers (tunneling devices) or paramagnetic metals (spin valves) are of major importance.

We investigate the ferromagnetic moment of CCFA at interfaces with Cr and AlO_x by polarised neutron reflectometry (PNR). Fitting the reflectometry data to a model which allows layers of the CCFA with different magnetic moments compared to the bulk moment, evidence for a reduced moment in a 1-2nm interface layer of the CCFA was identified. However, the reduction is clearly smaller at the Cr interface compared to the AlO_x interface.

Additionally, at the Cr interface the best fits are obtained, if ferromagnetic order of the complete 6nm Cr layer is assumed (with $\simeq 0.3\mu_B$/Cr-atom). This surprising observation is discussed in the framework of epitaxially induced stress of the Cr layer.

DS 41: Layer Deposition Processes

Time: Friday 14:30–16:00 Location: H 2032

DS 41.1 Fri 14:30 H 2032

On the correlation between process parameters and deposition rate in High Power Pulsed Magnetron Sputtering (HPPMS) discharges — •Dominik Koehl and Matthias Wuttig — I. Institute of Physics IA, RWTH Aachen University

In recent years, High Power Pulsed Magnetron Sputtering (HPPMS) has increasingly attained the focus of actual research on modern sputter deposition techniques. Due to its potential to apply an extremely high peak power to the sputter target, it enables thin film deposition with a very high degree of ionization of the sputtered material. The generation of a large amount of low energy ions in the plasma facilitates the possibility to tailor film properties by ion bombardment in a very wide range. Several authors have demonstrated e.g. the deposition of metal films showing an increased mass density and reduced surface roughness compared to the respective dc-sputtered films. Despite these and other promising advantages of HPPMS, its application for large scale industrial processes is still limited. This is mainly due to the fact that the deposition rates in many cases are reported to be significantly smaller than in dcMS at identical average powers or currents, so that the energy efficiency of the process is considerably reduced. This finding has been correlated to self-sputtering and gas rarefaction, which in turn has been attributed to the very high peak current during the pulse. We present a study that facilitates the development of a more fundamental understanding of the deposition rate with respect to several process parameters.

DS 41.2 Fri 14:45 H 2032

Magnetoelectrodeposition of CoFe — •Koza Jakub, Uhlemann Margitta, Gebert Annett, and Schultz Ludwig — IFW-Dresden, Dresden, Germany

The effect of a uniform magnetic field with flux density up to 1 T and different configuration on the electrodeposition of CoFe from simple sulphate electrolyte has been investigated. Voltammetric and chronoamperometric experiments have been carried out coupled with the electrochemical quartz crystal microbalance for the in situ mass measurements. The structure and morphology were determined by scanning electron microscopy, atomic force microscopy and X-ray diffraction measurements and the magnetic properties by VSM and MFM measurements. Results show that when the magnetic field is applied parallel to the electrode surface the limiting current density and deposition rate are increased due to the MHD-effect. The nucleation process is also affected in parallel configuration; this effect is attributed to hydrodynamic response of the electrochemical system. No significant influence on electrochemical reaction was observed when magnetic field was applied perpendicular to electrode. But in this configuration morphology and magnetic properties of deposited layers are changed by the magnetic field.

DS 41.3 Fri 15:00 H 2032

Interface roughness of MgO/Ti and ZrO_2/Ti multilayers — •Tobias Liese, Andreas Meschede, and Hans-Ulrich Krebs — Institut für Materialphysik, Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen

MgO/Ti and ZrO_2/Ti multilayers with double layer periods in the nanometer range were deposited by pulsed laser deposition (PLD) on Si(111) substrates in ultrahigh vacuum. The roughness of these films was investigated by atomic force microscopy (AFM), X-ray reflectometry (XRR), and transmission electron microscopy (TEM), which are sensitive on the surface and interface roughness, respectively. In both cases, the Ti layer grows in island growth, while the layer-by-layer growth of MgO and ZrO_2 layers leads to a smoothening of the layers. Therefore, with increasing number of bilayers no cumulative roughness is observed. The interfaces were studied by *in-situ* deposition rate and stress measurements. In this contribution, the underlying growth processes and their influence on the interface roughnesses are discussed.

DS 41.4 Fri 15:15 H 2032

Investigation of the Nucleation and Growth Mechanisms of Nanocrystalline Diamond Films — •Christian Sippel[1], Cyril Popov[1], Wilhelm Kulisch[2], Dieter Grambole[3], and Johann Peter Reithmaier[1] — [1]Universität Kassel, Institut für Nanotechnologie und Analytik, Heinrich-Plett-Straße 40, 34132 Kassel, Germany — [2]European Commission Joint Research Centre, Institute for Health and Consumer Protection, TP 203, Via Enrico Fermi 1, 21020 Ispra, Italy. — [3]Forschungszentrum Dresden-Rossendorf e. V., Institute of Ion Beam Physics and Materials Research, P. O. Box 510119, D-01314 Dresden, Germany

Nanocrystalline diamond (NCD)/ amorphous carbon composite films were deposited on Si substrates from CH_4/N_2 gas mixtures by microwave plasma chemical vapor deposition. Scanning electron microscopy (SEM), atomic force microscopy (AFM), Raman and Fourier transformed infrared (FTIR) spectroscopies, and nuclear reaction analysis (NRA) were applied to characterize the films. Ultrasonic pretreatment of the substrates with NCD powder suspended in n-pentane leads to nucleation densities on the order of $10^8\,cm^{-2}$; the variation of the grain size from 1 μm to 250 nm brings only marginal changes. In contrast, the addition of ultradispersive diamond powder increases the nucleation density by two orders of magnitude. Once the films are closed, their surface consists of larger features whose substructure is composed of much smaller features as revealed by SEM and AFM. The results from FTIR and NRA elucidate the complex mechanisms of hydrogen incorporation in the films and its role in the growth mechanism.

DS 41.5 Fri 15:30 H 2032

Rapid metal-sulphide-induced crystallization of highly textured tungsten disulphide thin films. — •Stephan Brunken[1], Rainald Mientus[2], and Klaus Ellmer[1] — [1]Hahn-Meitner-Institut, Glienicker Straße 100, 14109 Berlin — [2]Optotransmitter-Technologie-Umweltschutz e.V., Köpenicker Straße 325b, 12555 Berlin

Highly (001) textured tungsten disulphide (WS_2) thin films are grown by rapid metal(Co, Ni, Pd)-sulfide-induced crystallization of amorphous reactively sputtered sulphur-rich tungsten sulphide (WS_{3+x}) films. The rapid crystallization is monitored by real-time in-situ energy dispersive X-ray diffraction (EDXRD). Provided that a thin metal film is deposited prior the deposition of WS_{3+x} the films crystallize very fast (about 20 nm/s). The crystallization starts in the range of the Ni-S eutectic temperature of 637 °C. After crystallization isolated MeS(Me = Co, Ni, Pd)-crystallites are located on the surface of the WS_2-layer, which is proved by scanning electron microscopy and transmission electron microscopy. Taking into account the crystallization temperature this leads to the model of the rapid crystallization from liquid MeS_x droplets, which dissolve WS_x, oversaturate, release WS_2 while floating on the top of the crystallizing volume to the top of the layer. These metal-sulphide-induced crystallized $WS_2$2-layers exhibit a pronounced (001) orientation with large crystallites up to 3 μm. They show photoactivity and high hole mobilities (about 50 cm^2/Vs). Combined with the high absorption coefficient of 10^5 cm^{-1} and a direct band gap of 1.8 eV these properties make such films suitable for absorber layers in thin film solar cells.

DS 41.6 Fri 15:45 H 2032

Preparation of $CuInS_2$ chalcopyrite films by reactive magnetron sputtering: Influence of the Particle Energy on morphological, electrical and optical properties — •Stefan Seeger and Klaus Ellmer — Hahn-Meitner-Institut, Dep. Solar Energetics, Glienicker Str. 100, 14109 Berlin

Today magnetron sputtering is a common technique for large area depositions and already used to fabricate layers for thin film solar cells: the back contact (molybdenum) and front contact (zinc oxide) or for the deposition of metallic precursors. Nevertheless it is astonishing that this technique is not yet used for preparing the absorber layer in photovoltaic devices. Recently we have demonstrated that reactive magnetron sputtering from an indium and a copper target in an Ar/H_2S atmosphere is suited to prepare $CuInS_2$ absorber films and solar cells with an efficiency of more than 10% in a one-step process without additional annealing procedures. In order to make full use of the advantages of a plasma-assisted deposition process:
i) deposition at lower temperatures compared to pure thermal processes,
ii) high chemical reactivity,
iii) compact and well adherent films,
we have investigated in this work the influence of the particle energies on the film growth and the electronic properties.

DS 42: Layer Growth: Evolution of Structure and Simulation

Time: Friday 16:15–17:15 Location: H 2032

DS 42.1 Fri 16:15 H 2032

Numerical simulation of demixing of a binary mixture on the solid substrate with a free surface — •Lubor Frastia[1] and Len M. Pismen[2] — [1]MPG PKS, Nöthnitzer Straße 38, 01187 Dresden, Germany — [2]Dept. of Chemical Engineering, Technion, 32000 Haifa, Israel

The problem of simultaneous demixing and dewetting is frequently occuring in nano-technological applications, where the thickness of the internal interfaces in the phase-separated liquid may be comparable to the droplet size or layer thickness. Theoretical approaches to the demixing problem are commonly based on the Cahn–Hilliard theory [1] using the Landau–Cahn free energy functional approximation to model phase separation while neglecting the effects of the moving surfaces [2].

In this contribution, we describe the static limit of the model, given in [3], specialized for a 2D film lying on a solid substrate. Based on this model, we derived the Finite Element (FE) numerical procedure and computed droplet solutions for selected parameters of the model, using a continuation procedure with surface tension of the free surface, γ, as the continuation parameter. Resulting solution branch is compared with the related circular-symmetric droplet solution and its effective sharp interface approximation.

References:

1. J.W. Cahn and J.E. Hilliard, J. Chem. Phys. **28**, 258–267 (1958).

2. H.P. Fischer, P. Maass, and W. Dieterich, Europhys. Lett. **42**, 49–54 (1998).

3. U. Thiele, S. Madruga, L. Frastia, submitted to Physics of Fluids.

DS 42.2 Fri 16:30 H 2032

Molecular dynamics simulation study of the silicon carbide precipitation process — •Frank Zirkelbach[1], Jörg K. N. Lindner[1], Kai Nordlund[2], and Bernd Stritzker[1] — [1]Experimentalphysik IV, Institut für Physik, Universität Augsburg, Universitätsstr. 1, D-86135 Augsburg, Germany — [2]Accelerator Laboratory, Department of Physical Sciences, University of Helsinki, Pietari Kalmink. 2, 00014 Helsinki, Finland

The precipitation process of silicon carbide in heavily carbon doped silicon is not yet understood for the most part. High resolution transmission electron microscopy indicates that in a first step carbon atoms form C-Si dumbbells on regular Si lattice sites which agglomerate into large clusters. In a second step, when the cluster size reaches a radius of a few nm, the high interfacial energy due to the SiC/Si lattice misfit of almost 20A molecular dynamics simulation approach is used to gain information of the precipitation process on the atomic level. A newly parametrized Tersoff like bond-order potential is used to model the system appropriately. The present work discusses the first results gained by the molecular dynamics simulation.

DS 42.3 Fri 16:45 H 2032

Monitoring quantum dot growth by in-situ cantilever systems — •yan wang[1,2], huiling duan[1,2], and joerg weissmueller[1,3] — [1]Institute of Nanotechnology, Forschungszentrum Karlsruhe, Postbox 3640, Karlsruhe, 76021, Germany — [2]College of Engineering, Peking University, Beijing, 100871, P. R. China — [3]Technische Physik Universität des Saarlandes, 66041 Saarbruecken, Germany

There exist many theoretical and experimental works that focus on understanding the growth mechanisms of quantum dots (QDs). Without an in-situ measurement technique that monitors the growth modes of QDs such as the Frank-van der Merwe (FM), the Volmer-Weber (VW), the Stranski-Krastanow (SK) growth modes, and their corresponding ripening states during deposition, it is difficult to make conclusions on the growth mechanisms and on the ripening mechanisms of QDs. To monitor the growth modes, QDs are located on a MBE chamber equipped with an in-situ cantilever measurement setup, and this cantilever is used as a substrate of QD growth.

In this paper, based on continuum models, we investigate a series of problems related to the strained heteroepitaxial in-situ cantilever systems of QD growth.We first obtain the curvature of this cantilever system, which provides a way to monitor the possible growth modes (FM, VW, SK and their corresponding ripening states) in terms of island density, wetting layer thickness and cantilever thickness, etc. Then, we give the equilibrium conditions for SK growth, which provide the theoretical basis to control the sizes and the shapes of QDs. Finally, we simulate the morphological evolution of SK system.

DS 42.4 Fri 17:00 H 2032

Does ion beam divergence affect pattern formation by surface sputtering? — •Taha Yasseri[1], Emmanuel O. Yewande[2], Alexander K. Hartmann[3], and Reiner Kree[1] — [1]Institute for Theoretical Physics, University of Göttingen, Friedrich-Hund Platz 1, D-37075 Göttingen, Germany. — [2]Department of Computing and Mathematics, Manchester Metropolitan University, John Dalton Building, Chester Street, Manchester M1 5GD, United Kingdom — [3]Institut for Physics, University of Oldenburg, Carl-von-Ossietzky Strasse 9-11, 26111 Oldenburg, Germany.

In recent works on creating patterns like quantum dots or ripples via ion-beam surface sputtering, the importance of beam divergence for the creation of clear patterns is emphasized. Motivated by these experiments, we perform a (2+1)- dimensional Monte Carlo simulations of surface sputtering to study the influence of beam divergence on dynamics of pattern formation. We explain our results using linear continuum theory via evaluating the rate of growth for different modes. Generally beam divergence leads to a combination of different growth rates which slows down pattern formation. We find two exceptional situations where ion beam divergence may improve the quality of patterns. (1) Ion incidence perpendicular to the surface and (2) ion incidence around the critical angle where the orientation of formed ripples changes by 90 degrees. In case (1) anisotropic beam profiles with divergence may lead to ripples whereas isotropic profiles mainly affect the length scale of the formed dots. In case (2) non-zero beam divergence leads to patterns consisting of crossed ripples.